Binding energies of excitons and donors in a double quantum well in a magnetic field

J. Cen and K. K. Bajaj
Department of Physics, Emory University, Atlanta, Georgia 30322
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We study binding energies of both excitons and donors in a symmetric double quantum well in the presence of a magnetic field applied parallel to the growth direction. We express wave functions as combinations of Gaussian-type orbitals and subband wave functions of even and odd parities, with variationally determined expansion parameters. By varying the interwell barrier width and well sizes (hence varying the interwell coupling), we obtain binding energies ranging in character from that for a strongly coupled double well to that for a system of two isolated single wells. The behavior of the binding energies as function of the interwell coupling, well sizes, and the magnetic field, as well as the donor position is consistently described with our formalism with naturally included subband mixing effects. The magnetic field leads to stronger confinement of the wave functions and enhances binding energies.

I. INTRODUCTION

Double quantum-well structures have attracted a good deal of attention, both experimentally and theoretically.[1-7] A double quantum well (DQW) is a semiconductor structure in which two single quantum wells are separated by only a thin potential barrier, across which electrons and holes from one well can tunnel into the other. As in single quantum wells, the electrons and holes confined in a DQW can form excitons due to their mutual Coulomb attraction. The electro-optical properties of such excitons promise applications in high-speed spatial-light modulators and switches.[8] One advantage that a DQW structure offers over the single quantum wells is the enhanced exciton electro-optic response.[9]

A magnetic field applied parallel to the growth direction has an additional confining effect on electrons and holes in the quantum wells, and is expected to modify exciton binding energies in the DQW.[10-12] Together with effects of the confinement and interwell coupling (through tunneling across the potential barrier) provided by a DQW, we have an interesting physical system in which these competing factors influence those exciton characteristics determining the exciton electro-optical properties of the DQW. Although several authors have done a considerable amount of work on the properties of excitons in DQW's,[13-16] to our knowledge the effects of a magnetic field on DQW's have not been theoretically studied. In addition, there are some conflicting results obtained by these various authors as to how interwell coupling would qualitatively affect exciton binding energies in a DQW in the weak and strong interwell coupling limits. A qualitative and quantitative study is desired to gain knowledge of these aspects and to clear up ambiguities about the role played by interwell coupling in affecting exciton binding energies in a double quantum well.

In the presence of a hydrogenic donor impurity, the Coulomb interaction of the donor with an electron in the DQW leads to the formation of hydrogenic bound states and the removal of the reflection symmetry. Optical transitions involving donor states in quantum-well structures have attracted interest for some years.[17-21] The binding energies of hydrogenic donors in quantum-well structures have been calculated by various authors.[17,22-31] Because a symmetric DQW with a varying center potential barrier thickness (or height) can range in character from a double-width well to a pair of decoupled single wells, a potentially rich spectrum of physics can arise from the competing effects of quantum confinement and tunneling in this structure. Such a DQW structure with wide-ranging characteristics, however, also demands a more careful approach for one to describe consistently the physical processes taking place in it. Electron wave function tends to pile up around a positively charged donor atom due to the Coulomb attraction. Depending on the donor location, electron wave function in the symmetric quantum-well structure can be highly asymmetrical. A single-subband treatment using a definite parity subband wave function can be inadequate in such instances to describe the electron charge distribution around the donor, and can lead to a lower estimate of the binding energy even for thin barrier thicknesses. Inclusion of such mixing plays an important role in correctly determining donor binding energies in a symmetric quantum-well structure.

Subband mixing is ignored in the few treatments in the present literature dealing with donor binding energies in symmetric DQW structures. Chen and Zhou[7] considered the problem of donor binding energy in a symmetric double quantum well with the donor atom located within the center barrier. Product of the lowest (even-parity) subband wave function and a variational hydrogenic wave function was used to obtain the donor binding energies for various symmetric DQW structures. These authors, however, are unable to recover the corresponding single-well limits when the center potential barrier becomes very thick.

It is now clear that such a single-subband approach cannot recover the single-well limit as barrier thickness increases. The basic reason is simply as follows. Tunneling across the potential barrier becomes increasingly less

probable as the barrier thickness increases. Not able to penetrate the potential barrier, an electron will be essentially confined in one single well. Ignoring subband mixing, however unrealistically, forces the electron wave function to spread throughout DQW structure, which reduces the probability of finding an electron in the vicinity of the donor, and therefore reduces the donor binding energy.

In this paper we develop a formalism to calculate the binding energies of excitons and donors in DQW structures, with effects of subband mixing included, in the presence of a magnetic field directed along the growth axis. The formalism is applied to a GaAs-$Al_xGa_{1-x}As$ DQW for various physical parameters. The preliminary results in the case of the exciton binding energies were first presented at the 1991 March Meeting of the American Physical Society.[32] In Sec. II, we describe this formalism, in which we solve for electron and hole wave functions in the double-well potential profile; take mixing of electron and hole wave functions of neighboring subbands into account; express the electron-hole and electron-donor internal-state wave function in terms of Gaussian-type orbitals and determine expansion parameters and exciton binding energies variationally. In Sec. III we show that our formalism correctly describes exciton and donor binding energies for all interwell coupling strengths, and discuss the binding energies as a function of the quantum confinement, the magnetic field, and the interwell coupling.

II. FORMALISM

We consider a DQW consisting of two identical GaAs layers sandwiched between two semi-infinite $Al_xGa_{1-x}As$ slabs, with a thin layer of $Al_{x'}Ga_{1-x'}As$ between them. A uniform magnetic field **B** is applied perpendicular to the layers (in the growth direction).

The Hamiltonian of the electron-hole system is[33]

$$H=H_e\left[-i\hbar\nabla+\frac{e}{c}\mathbf{A}\right]-H_h\left[i\hbar\nabla+\frac{e}{c}\mathbf{A}\right]+V_e(z_e)+V_h(z_h)-\frac{e^2}{\kappa_0|\mathbf{r}_e-\mathbf{r}_h|}\ , \tag{1}$$

where $V_e(z)$ and $V_h(z)$ are, respectively, the potential profiles for the electrons and holes, $\mathbf{A}=(\mathbf{B}\times\mathbf{r})/2$ is the vector potential of the magnetic field **B**, κ_0 is the dielectric constant of the layers (assumed to be uniform here), $\mathbf{r}_e$ and $\mathbf{r}_h$ are the electron and hole positions. The electron Hamiltonian H_e is adequately described by an effective-mass approximation, using parabolic bands. The hole Hamiltonian H_h is the 4×4 Kohn-Luttinger Hamiltonian.[34] To gain physical insight with a tractable model, we assume parabolic hole bands in the x-y plane and in the z direction and retain only the diagonal terms in H_h, thereby ignoring coupling between the heavy-hole and light-hole bands. Following standard procedure to separate the constant center-of-mass motion of an electron-hole pair in the x-y plane, we define the reduced mass of an electron-hole pair μ with $\mu^{-1}=m_e^{-1}+(\gamma_1\pm\gamma_2)m_0^{-1}$, where m_0 is the free-electron mass, m_e is the effective electron mass, and γ_1 and γ_2 are the Kohn-Luttinger band parameters, the + sign corresponds to the heavy-hole exciton, and the − sign to the light-hole exciton. We then scale all lengths in the exciton Bohr radius $a_B=\kappa_0\hbar^2/\mu e^2$, and energies in the exciton Rydberg $R=e^2/2\kappa_0 a_B$, to obtain the dimensionless form of the Hamiltonian

$$H=-\left[\frac{\partial}{\rho\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{\partial^2}{\rho^2\partial\varphi^2}\right]+H_e'(z_e)+H_h'(z_h)-\frac{2}{\sqrt{\rho^2+z^2}}+\gamma L_z+\frac{\gamma^2}{4}\rho^2\ , \tag{2}$$

where $\rho=\sqrt{(x_e-x_h)^2+(y_e-y_h)^2}$ is the in-plane distance between a pair of electron and hole, $z=z_e-z_h$, L_z is the z component of the angular momentum, and γ is the first Landau level expressed in R, $\gamma=e\hbar B/2\mu cR$. The Hamiltonian H above is grouped into three terms, namely the electron part H_e', the hole part H_h', and the exciton part $H_{\rm ex}^B$, $H=H_e'+H_h'+H_{\rm ex}^B$, where

$$H_e'(z_e)=-\frac{\mu}{m_e}\frac{\partial^2}{\partial z_e^2}+V_e(z_e)\ , \tag{3a}$$

$$H_h'(z_h)=-\frac{\mu}{m_h}\frac{\partial^2}{\partial z_h^2}+V_h(z_h)\ , \tag{3b}$$

$$H_{\rm ex}^B=\left\{-\left[\frac{\partial}{\rho\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{\partial^2}{\rho^2\partial\varphi^2}\right]-\frac{2}{\sqrt{\rho^2+z^2}}\right\}+\gamma L_z+\frac{\gamma^2}{4}\rho^2\ , \tag{3c}$$

and m_h is the heavy- (light-) hole mass defined in $m_h^{-1}=(\gamma_1\mp2\gamma_2)m_0^{-1}$. The Hamiltonian in Eq. (2) reduces to that for an electron bound to an immobile donor if we replace $\mathbf{r}_h$ with position of the donor $\mathbf{r}_d$ and set $V_h(z_h)$, γ_1, and γ_2 equal to zero (which corresponds to infinite hole masses).

Wave function $\psi(\mathbf{r}_e,\mathbf{r}_h)$ of the electron-hole system is solved from the Schrödinger equation

$$H\psi(\mathbf{r}_e,\mathbf{r}_h)=E\psi(\mathbf{r}_e,\mathbf{r}_h)\ , \tag{4}$$

where E is the total energy. We write $\psi(\mathbf{r}_e,\mathbf{r}_h)$ in the following form to express the explicit dependence on z_e, z_h and on the relative distance $\mathbf{r}=\mathbf{r}_e-\mathbf{r}_h$:[35]

$$\psi(\mathbf{r}_e,\mathbf{r}_h)=\phi(\mathbf{r})\sum_{k=1}a_kF_e^k(z_e)\sum_{l=1}b_lF_h^l(z_h)\ , \tag{5}$$

where $\phi(\mathbf{r})$ is the wave function describing the internal state of an exciton, $F_e^k(z_e)$ is the kth electron subband wave function, and $F_h^l(z_h)$ the lth hole subband wave function, a_k and b_l are the expansion coefficients to be determined, both $F_e^k(z_e)$ and $F_h^l(z_h)$ are normalized. In the calculation of the donor binding energies $|F_h(z_h)^2|\rightarrow\delta(z_h-z_d)$. Equation (5) is a good approximation to the exciton wave function, as long as the difference between the subband levels that are included in the summation and those that are not is larger than the exciton binding energies. The two wave functions in the z direction are determined by the following two equations:

$$H_e' F_e^k(z_e) = E_e^k F_e^k(z_e) \ , \tag{6a}$$

$$H_h' F_h^l(z_h) = E_h^l F_h^l(z_h) \ , \tag{6b}$$

in which E_e^k and E_h^l are the electron and hole subband energies.

We first solve for the subband envelope functions $F_e(z_e)$ and $F_h(z_h)$. Since H_e', and H_h' have the same form, we can solve the general double-well problem for the following profile $V(z)$;

$$V(z) = \begin{cases} V_w \ , & |z| > z_2 \\ 0 \ , & z_1 < |z| < z_2 \\ V_b \ , & |z| < z_1 \ , \end{cases} \tag{7}$$

where $z_1 = L_b/2$, $z_2 = z_1 + L_w$, L_b is the width of the center potential barrier, L_w is the width of a single quantum well, V_b is the center barrier height, V_w is outer potential wall height. We write $F(z)$ in the following form to reflect the symmetry of $V(z)$:

$$F(z) = \begin{cases} D \exp[-\beta_2(z - z_2)] \ , & z > z_2 \\ A \sin[\alpha(z - z_1)] + B \cos[\alpha(z - z_1)] \ , & z_1 < z < z_2 \\ 2C\chi_{\pm}(\beta_1 z) \quad |z| < z_1 \\ \mp A \sin[\alpha(z + z_1)] \pm B \cos[\alpha(z + z_1)] \quad -z_2 < z < -z_1 \\ \pm D \exp[\beta_2(z + z_2)] \ , & z < -z_2 \ , \end{cases} \tag{8}$$

where $+$ indicates the wave function $F(z)$ as being of even parity, $-$ as being of odd parity, α, β_1, and β_2 are the parameters determined by the subband energy E_σ, $\alpha = \sqrt{m_\sigma E_\sigma}/\mu$, $\beta_1 = \sqrt{m_\sigma |V_b^\sigma - E_\sigma|}/\mu$, $\beta_2 = \sqrt{m_\sigma (V_w^\sigma - E_\sigma)}/\mu$, $(\sigma = e, h)$, and

$$\chi_{\pm}(\beta_1 z) = \begin{cases} \cosh\beta_1 z \quad (+) \\ \sinh\beta_1 z \quad (-) \ , \quad V_b > E \\ \cos\beta_1 z \quad (+) \\ \sin\beta_1 z \quad (-) \ , \quad V_b < E \ . \end{cases} \tag{9}$$

By requiring the continuity of $F(z)$ and $\partial F(z)/\partial z$ at interfaces $z = \pm z_1$ and $z = \pm z_2$, we obtain the secular equation for the subband energy $E_{e(h)}$,

$$\left[\beta_2 \frac{\partial \chi_{\pm}(\beta_1 z_1)}{\partial z_1} - \alpha^2 \chi_{\pm}(\beta_1 z_1)\right] \sin\alpha L_w + \alpha \left[\frac{\partial \chi_{\pm}(\beta_1 z_1)}{\partial z_1} + \beta_2 \chi_{\pm}(\beta_1 z_1)\right] \cos\alpha L_w = 0 \ . \tag{10}$$

After the subband energy is obtained, coefficients A, B, C, and D for the wave function $F(z)$ are then determined by the continuity and normalization conditions. The wave function of the lowest subband is of even parity, that of the second subband is of odd parity.

Next we express the exciton internal-state wave function $\phi(\mathbf{r})$ in terms of Gaussian-type orbitals and use a variational calculation to determine the expansion parameters and the exciton binding energy.

$$\phi(\rho, \varphi; z) = \frac{e^{im\varphi}}{\sqrt{2\pi}} \rho^{|m|} e^{-\beta\rho^2} \sum_{j=1}^{n} c_j \exp[-\alpha_j(\rho^2 + z^2)] \quad (m = 0, \pm 1, \pm 2, \ldots) \ , \tag{11}$$

where β is the variational parameter, c_j are the expansion coefficients, α_j are sets of constants.[36,37] m is the azimuthal quantum number; for the $1s$ state, $m = 0$; for the $2p_{\pm}$ states, $m = \pm 1$; and so on. For excitons in the double quantum well, β is varied to adjust these Gaussian-type basis functions to minimize the total energy E.

For DQW's consisting of narrow wells with strong interwell couplings (for center barriers of small widths or low heights), effects of the coupling between neighboring subbands on exciton binding energies are shown to be small; therefore it is sufficient to assume the exciton to be associated with a single electron subband and a single hole subband.[17] In general, however, the single-subband description of an exciton in a double quantum well is inadequate and can lead to qualitatively misleading results. When two single quantum wells are separated by a potential barrier, the wave functions in these wells are scrambled to form a "bonding" (even-parity) and an "antibonding" (odd-parity) combination (total) wave function. If the barrier is thin *and* the wells are narrow, the single-well wave functions are strongly modified by the presence of the neighboring well because of the tunneling of the electron (hole) across the potential barrier. As a result, the bonding and antibonding total wave functions have significantly different subband levels. In other words, subband levels in such a thin-barrier, narrow-well DQW are nondegenerate. When the barrier is thicker *or* the wells are wider, single-well wave functions are essentially confined to one single well and are therefore diminishingly affected by the presence of its neighboring well. Bonding and antibonding combinations would yield similar subband levels, with one slightly lower and one slightly higher than the isolated single-well subband levels. All subband levels are *almost* doubly degenerate. A consistent description of exciton in DQW structures should therefore include *pairs* of subband levels to properly account for contributions to exciton binding energies from both the even-parity and odd-parity subband wave functions. In the case of an electron bound to the donor, the electron system no longer has a definite symmetry, and neither the even- nor the odd-parity wave function alone can be the true wave function. We take a linear combina-

tion of the wave functions of different subbands as the envelope function.

In what follows, we calculate the binding energies of the $1s$ exciton state associated with the first two electron and hole subbands and binding energies of the $1s$ and $2p$ donor states associated with the first two electron subbands. In a system with thin barrier and narrow wells, the separation between the adjacent subband levels are large compared with the expected exciton binding energies and there is little intersubband coupling, i.e., $a_1 b_1 \approx 1$ and $a_k b_l \to 0 (k+l>2)$. As $L_b \to \infty$, these subband levels become degenerate and coupling between them becomes important, i.e., all a_k and b_l would play comparable roles. In the absence of the Coulomb interaction and without mixing of the even-parity and odd-parity subbands, the total energy E is just the sum of first electron and hole subband energies $E_e^{(1)}$, $E_h^{(1)}$ and the Landau-level energy γ. The Coulomb interaction between the electron and hole lowers the total energy and leads to the formation of the exciton. The binding energy of the lowest-lying exciton E_B is defined in $E_B = E_e^{(1)} + E_h^{(1)} + \gamma - E$. Similarly, binding energies of the $1s$ and $2p_-$ donor states is $E_B = E_e^{(1)} + \gamma - E$. Binding energies of the $2p_+$ state can be obtained by simply adding 2γ to the $2p_-$ state values.

The total energy E is obtained by expressing the Schrödinger equation (4) as an eigensystem problem with the nonorthogonal Gaussian-type orbitals as basis functions, which is then solved by a generalized Rayleigh quotient iteration method.[38] By choosing the appropriate eigenvalue λ and minimizing it as a function of the variational parameter, we obtain the total energy E of a given exciton/donor state and its binding energy E_B.

III. RESULTS AND DISCUSSION

A. Exciton binding energies

We have calculated the binding energies of the heavy-hole exciton and the light-hole exciton as functions of the magnetic field, the well width L_w, and the center barrier thickness L_b of a symmetric GaAs-$Al_xGa_{1-x}As$ double quantum well. The values of physical parameters pertaining to GaAs used in our calculations are $m_e = 0.067 m_0$, $\kappa_0 = 12.5$, $\gamma_1 = 7.36$, $\gamma_2 = 2.57$.[39] The values for the heavy-hole ($J_z = \pm\frac{3}{2}$) exciton are $m_h = 0.45 m_0$, $\mu = 0.04 m_0$, $a_B = 165$ Å, $R = 3.49$ meV; those for the light-hole ($J_z = \pm\frac{1}{2}$) exciton are $m_h = 0.08 m_0$, $\mu = 0.05 m_0$, $a_B = 131$ Å, $R = 4.39$ meV. We use an empirical formula $\Delta E_g = (1.36 + 0.22x)x$ (eV) to determine the band-gap discontinuity,[40] with 60% of ΔE_g contributing to the conduction-band discontinuity ΔE_c and 40% to the valence-band discontinuity ΔE_v. Mole fraction $x = 0.3$ is used for all Al concentrations. Differences between other material parameters of GaAs and those of $Al_xGa_{1-x}As$ are not included in the calculations (see Fig. 1).

In Fig. 2, we compare the binding energies of the heavy-hole exciton in a DQW calculated by us, with those obtained by Kamizato and Matsuura (KM hereafter)[14] with and without subband mixing, and those by Dignam and Sipe (DS hereafter)[16] with subband mixing, as a function of the barrier thickness L_b. It is evident that the two-subband treatment by DS underestimates the binding energy in the strongly interwell coupling limit ($L_b \lesssim 0.2 a_B$) and cannot reconcile with the fact that, at $L_b = 0$, the DQW is simply a single well of width $2L_w$.

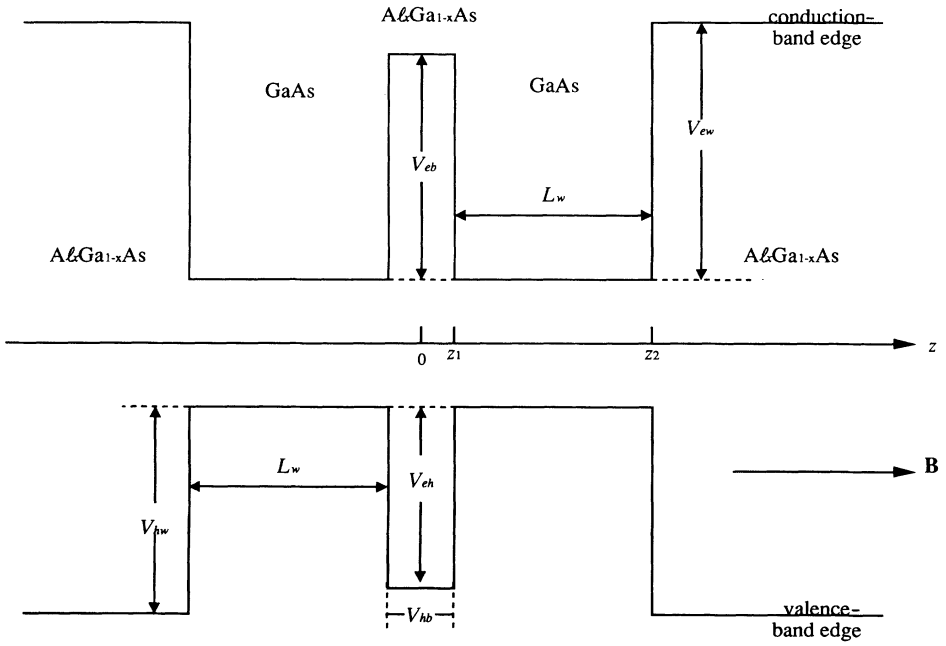

FIG. 1. Schematic band diagram of a symmetric GaAs-$Al_xGa_{1-x}As$ double quantum well and the applied magnetic field **B** in the growth direction.

On the other hand, the two-subband DS result in the weak interwell coupling limit approaches that obtained by KM without subband mixing, which cannot recover the single-well result at large barrier thicknesses either. It appears that although the DS two-subband treatment works at the intermediate interwell coupling strengths, it overestimates the strength of the interwell coupling in both the strong and weak interwell coupling limits. Our result agrees with that of KM, including subband mixing at both strong and weak interwell coupling limits. It is also evident that our formalism gives higher binding energies for all interwell coupling strengths. Furthermore our formalism correctly describes exciton binding energies when the additional confining effect of the magnetic field is also included.

In Fig. 3(a), we show variation of the binding energy E_B of the heavy-hole exciton as a function of well widths L_w for several different combinations of the barrier thickness L_b and the magnetic field B. The results of E_B for $L_b=0$ have been compared with those of Greene and Bajaj for exciton binding energies in a single quantum well in a magnetic field,[10] based on the expansion of the exciton wave function into Gaussian basis orbitals. These for zero magnetic field ($B=0$) and $L_b \ll a_B$ have been compared with the results obtained by KM for the exciton binding energies in a symmetric double quantum well, with material parameters roughly corresponding to those of heavy-hole excitons in GaAs-$Al_xGa_{1-x}As$ quantum wells.[14] The agreement in both cases is excellent, as expected.

For $L_b=0$, as well width L_w decreases, electron and hole wave functions first become compressed in the narrowing wells and the exciton binding energy E_B climbs up due to the decreasing average distance between the electron and the hole, which is mainly determined by the well size L_w and barrier thickness L_b in a given magnetic field, until E_B reaches a maximum. As L_w further decreases, subband energies are pushed up and leakage of the wave functions into the barrier regions becomes significant, and E_B begins to fall off rather rapidly as the exciton assumes more of a 3D-like nature.[35].

For $L_b \neq 0$, the binding energy is lower for small L_w and higher for large L_w, in comparison to that in the DQW with $L_b=0$. For narrow wells, the electron and hole wave functions spread throughout the DQW struc-

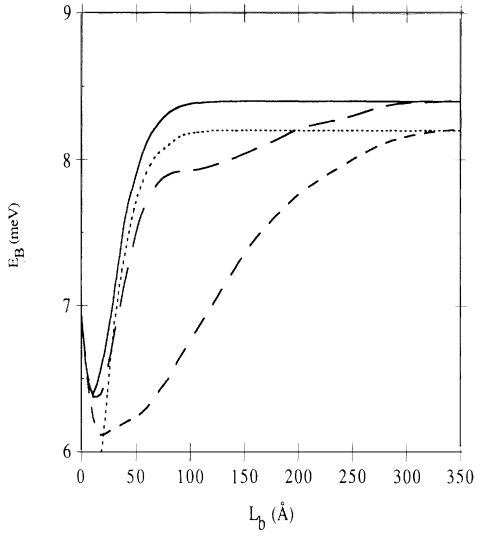

FIG. 2. Comparison of binding energies of the heavy-hole exciton, calculated with and without subband mixing, as a function of the barrier thickness L_b. The well width is fixed at $L_w=0.6a_B$. The solid line (——) is our result with subband mixing included; the dotted line (· · · ·) is by Dignam and Sipe (Ref. 16) with subband mixing; the short-dashed line (— — —) is by Kamizato and Matsuura (Ref. 14) without subband mixing; the long-dashed line (— —) is by Kamizato and Matsuura with subband mixing. The material parameters are as in Ref. 14.

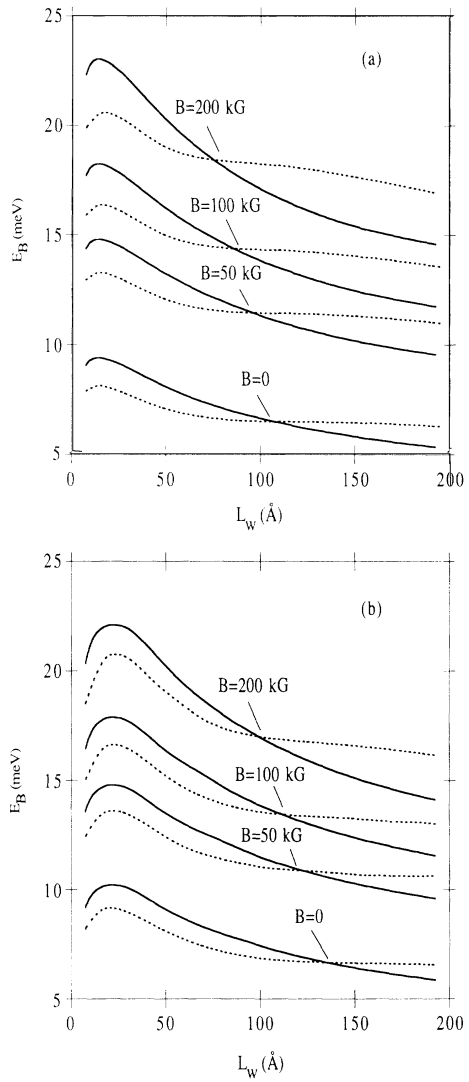

FIG. 3. (a) The binding energy of the heavy-hole exciton as a function of the well width L_w. (b) The binding energy of the light-hole exciton as a function of the well width L_w, with magnetic field B and barrier thickness L_b as the two other parameters. Material parameters are noted in text. The solid lines (——) stand for $L_b=0$ (corresponding to that in a single quantum well of width $2L_w$); the dotted lines (· · · ·) stand for $L_b=25$ Å.

ture, and the presence of the barrier merely increases the average distance between the electron and hole, leading to a lower binding energy. As the wells become wider, however, the wave functions become more and more confined in one single well due to the presence of the barrier, and the average distance between the electron and hole decreases, leading to a higher binding energy. At a well width L_w^c, the E_B curves in the DQW with $L_b \neq 0$ will cross over with that in the DQW with $L_b = 0$. Since a magnetic field provides an extra confinement of the wave function in the quantum well, such a crossover will occur at a smaller L_w^c at higher field strengths. Also notice that a shoulder develops in the binding-energy curves. As L_b increases, this shoulder will become more evident and appears at smaller well widths L_w. At the limit $L_b \rightarrow \infty$, it merges with the maximum that is caused by the leakage of lowest subband wave functions into the barrier regions. This shoulder is attributed to the mixing of wave functions of the odd-parity second subbands with those of the even-parity first subbands. For small L_b, $E^{(1)}$ and $E^{(2)}$ are significantly different, and wave functions of the second subbands are more spread out due to their higher energies. The binding energy influenced by the second subbands would reach its maximum at the large well width L_w. As L_b increases, the second subband lowers down and eventually becomes degenerate with the first subband, and the maximum in E_B caused by it coincides with that of the first subband.

In Fig. 3(b), we show values of the binding energy E_B of the light-hole exciton as a function of L_w. Qualitatively E_B behaves similar to the binding-energy of the heavy-hole exciton. However, it is larger and reaches the maximum for larger L_w compared to that of the heavy-hole exciton.[41] Also, the values of light-hole exciton binding energy are higher than those obtained by Greene and Bajaj, who used 85–15 % conduction-valence band offsets in their calculations,[10] as light holes are now more severely confined in the quantum wells by higher potential barriers. The binding energies of the heavy-hole exciton associated with the lowest subband are not as sensitive to the change of band offsets used in the calculations, since the heavier longitudinal mass results in stronger confinement of the heavy-hole wave function in the quantum wells. However, for excitons associated with higher subbands, higher valence-band offsets are expected to affect binding energies more significantly for both the light-hole and heavy-hole excitons. In all instances, the presence of a magnetic field in the growth direction leads to higher exciton binding energies. Our results on the heavy-hole exciton fit rather well with those measured by Perry *et al.*,[12] when appropriate material parameters are used in the calculations.

In Fig. 4(a), we show the binding energies of the heavy-hole exciton as functions of barrier thickness L_b for several different values of (L_w, γ). Similar results for the light-hole exciton are displayed in Fig. 4(b). At $L_b = 0$, results for single quantum wells of width $2L_w$ are recovered, as we have noted earlier. The average distance between the pair of electron and hole forming the exciton increases as L_b increases from zero, and as a result the binding energy E_B drops down first. For small barrier thicknesses, a significant portion of wave functions is present in the barrier regions. However, this leakage decreases sharply as well size increases.[35] Therefore for wider wells the rate at which the binding energy drops down as L_b increases is higher, as it is easier to separate the wave function in the two neighboring wells when the center barrier size L_b increases.

As L_b further increases, coupling between the well diminishes, and the binding energies will eventually climb up and approach the isolated single-well values $E_B(L_w)$. The E_B curves will bottom out at barrier thickness L_b and then rise up. Again for wider wells, this minimum in E_B will occur at smaller barrier thickness L_b. Notice also that as the magnetic field increases, the exciton wave

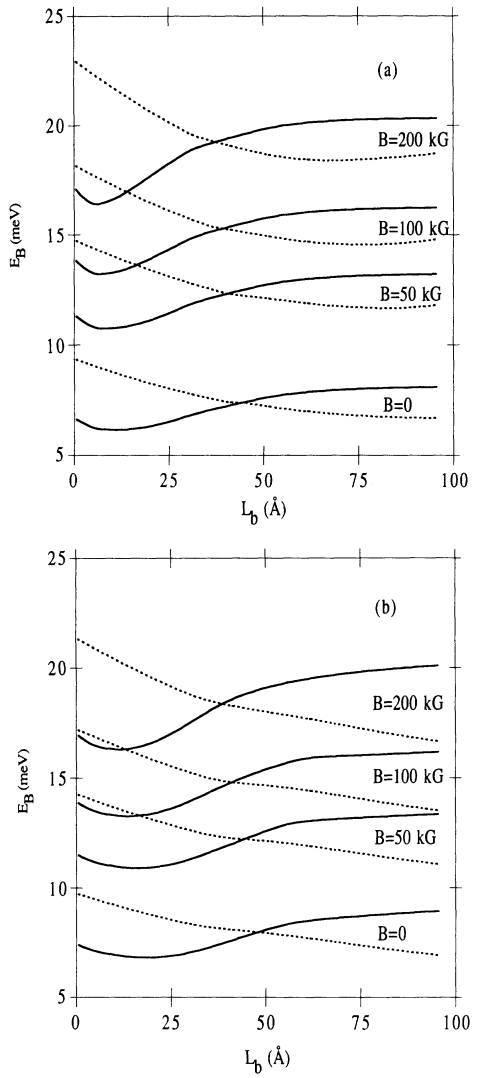

FIG. 4. (a) The binding energy of the heavy-hole exciton as a function of the barrier thickness L_b. (b) The binding energy of the light-hole exciton as a function of the barrier thickness L_b. The other two parameters are the magnetic field B and the well width L_w. Solid lines (——) stand for $L_w = 100$ Å; dotted lines (· · · ·) for $L_w = 10$ Å.

function spread is reduced, and as a result the interwell coupling decreases faster as the barrier thickness increases. The minimum of the binding energy occurs at smaller L_b.

It is worth pointing out that so far only our approach, to our knowledge, has produced consistent results for all barrier sizes. Although we have calculated only the binding energies of excitons associated with the first electron and hole subbands, our formalism here can be applied to excitons associated with other subbands.

B. Donor binding energies

We have also calculated the binding energies of the $1s$ and $2p_{\pm}$ donor states in symmetric double GaAs-$Al_xGa_{1-x}As$ quantum-well structures in a magnetic field. The effective Bohr radius $a_B = 99.5$ Å, and effective Rydberg $R = 5.79$ meV. Using only the lowest subband in our calculations, we easily recover for the $1s$ donor state in the case of zero magnetic field the results of Chen and Zou,[7] who used the even-parity lowest subband in their calculations of donor binding energies in a symmetric double quantum well.

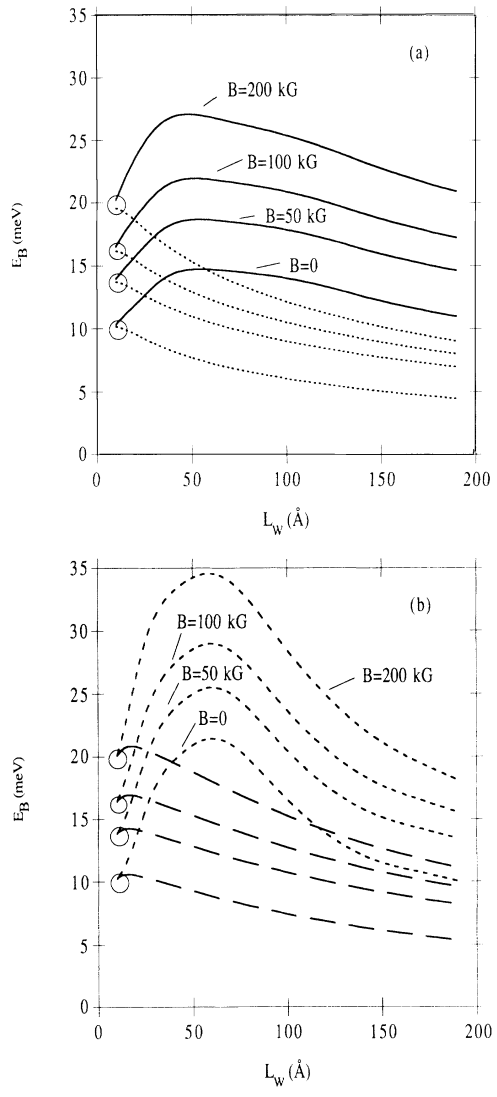

FIG. 5. The binding energy of the $1s$ donor state E_B as a function of well size L_w, for a fixed barrier thickness $L_b = 50$ Å, for several values of magnetic field B (kG). (a) The solid lines (——) stand for a well-center donor, the dotted lines (· · · ·) for a barrier-center donor. (b) The long-dashed lines (— —) stand for a barrier-edge donor, the short-dashed lines (– – – –) for an outer-well-edge donor.

In Fig. 5, we show the binding energy of the $1s$ state as a function of well size L_w. Four different cases are considered: (1) a barrier-center donor, (2) a barrier-edge (inner-well-edge) donor, (3) a well-center donor, and (4) an outer-well-edge donor. The center barrier thickness is fixed at $L_b = 50$ Å. The well size is varied from $L_w = 10$ to 200 Å. All four donor locations yield similar binding energies at small well widths. This is due to the fact that, since the electron wave function is spread throughout a narrow-well DQW structure, the probability of finding an electron in the vicinity of a randomly distributed donor is almost independent of the donor location. As well size increases, the binding energy of the barrier-center donor monotonically decreases, as the wave function becomes more and more concentrated inside the quantum well, increasing the average electron-donor distance. For the barrier-edge donor, however, it is possible that there exists a favorable probability of an electron being in the vicinity of the donor at some small L_w, since the electron wave function tends to pile up around a positive charge. A maximum in the binding energy exists at some small well sizes. As well size further increases, the elctron wave function is increasingly confined inside the well, and the binding energy then decreases due to the larger average electron-donor distance. For the well-center donor, the confinement of the electron wave function inside the well at increasing L_w strongly favors a larger binding energy. As well size further increases, the spread of the wave function in the well and surrounding regions reduces the probability of the electron staying close to the donor, and the binding energy decreases. For the outer-well-edge donor, the increasing confinement of the electron wave function to the inside of the well as L_w increases leads to higher binding energies at small well sizes, but eventually leads to a larger average electron-donor distance and hence to lower binding energies. Notice that the maximum binding energies of the donor at the outer-well edge are higher than those at the well center. This is attributed to a stronger mixing of the even- and off-parity DQW wave functions in the vicinity of the donor.

In Fig. 6, we show the $2p_-$-state binding energies as a function of well size L_w for a fixed barrier size $L_b = 50$ Å. For the $2p_-$ state, donors at all locations have lower binding energies than those of the $1s$ state because of the larger wave-function spread. The barrier-center and barrier-edge donor binding energies behave in a qualitatively similar way with their $1s$ counterparts. The behavior of the well-center and outer-well-edge binding energies of the $2p_-$ states, however, is qualitatively different from that of the $1s$ state for the following reason. In narrow quantum-well structures, the $2p_-$-state wave function is highly compressed, much more so than that of the

$1s$ state. As well size increases, the $2p_-$-state wave function is allowed to relax in the structure, both in the growth direction and in the x-y plane. For the well-center donor, such an expansion of the electron wave function reduces the probability of finding the electron in its vicinity, therefore its binding energy decreases. After the expansion is largely accomodated by even wider wells, the electron wave function tends to pile up around the donor and the binding energy will first increase to reach a maximum and then behave like that of the $1s$ state. For the outer-well-edge donor, the binding energy will initially also decrease. Since it is more sensitively affected by the spatial extent of the electron wave function, it recovers to a maximum at smaller well sizes and then drops down at a steeper rate as well size further increases.

Both $1s$- and $2p_-$-state binding energies in a magnetic field behave qualitatively like zero-field counterparts. In addition to giving higher binding energies, the stronger quantum confinement by the magnetic field also increases the rate at which the binding energies change at increasing well sizes.

In Fig. 7, we show binding energies of the $1s$ state as a function of barrier thickness L_b for a fixed well size $L_w = 50$ Å. As the barrier thickness increases, the barrier-center donor binding energy monotonically decreases, as the probability of finding the electron in its vicinity can only become more remote. The barrier-edge donor binding energy initially also decreases when L_b increases from zero, as the single-well (of width $2L_w$) wave function begins to separate and the probability of finding the electron in its vicinity decreases. As L_b further increases, however, the DQW wave function gradually becomes an effectively single-well wave function (with subband mixing), and the binding energy quickly recovers its value in a single quantum well of width L_w. It should be pointed out that a single-subband treatment will always assume comparable portions of the electron wave function in both wells, no matter how thick the barrier has become, and will therefore always underestimate donor binding energies in the symmetric DQW structure. The well-center donor starts out with roughly the same binding energies as the barrier-center and barrier-edge donors at small barrier thicknesses, since the binding energy is not very sensitive to changes in location for a donor not close to the surrounding potential walls in a single quantum well (size $\sim 2L_w$). This situation quickly changes as

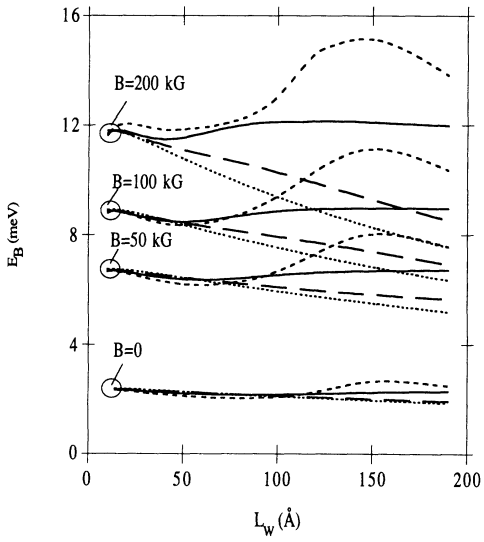

FIG. 6. The binding energy of the $2p_-$ donor state E_B as a function of well size L_w, for a fixed barrier thickness $L_b = 50$ Å, for several values of magnetic field B (kG). The solid lines (——) stand for the well-center donor, the dotted lines (· · · ·) for the barrier-center donor, the long-dashed lines (— —) for the barrier-edge donor, and the short-dashed lines (– – – –) for the outer-well-edge donor.

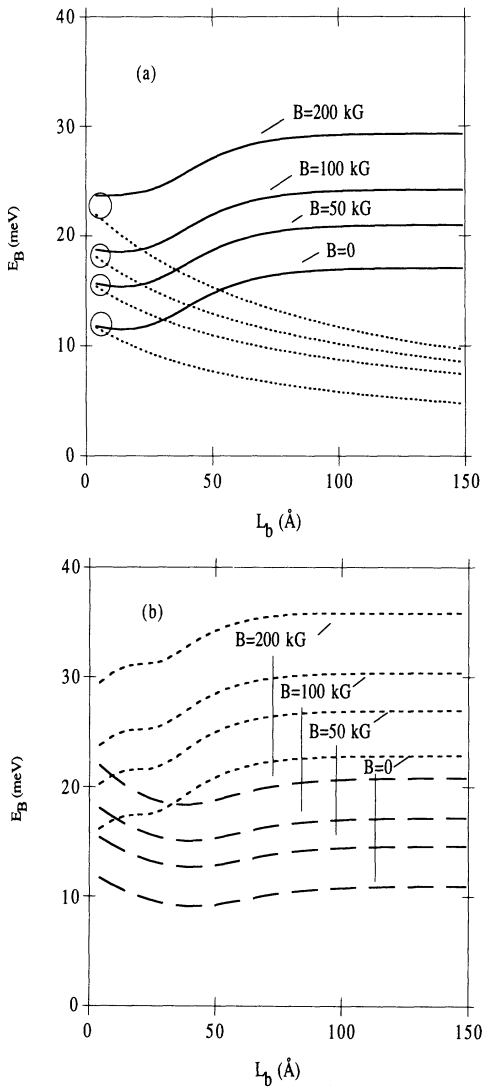

FIG. 7. The binding energy of the $1s$ donor state E_B as a function of barrier thickness L_b, for a fixed well size $L_w = 50$ Å, for several values of magnetic field B (kG). (a) The solid lines (——) stand for the well-center donor and the dotted lines (· · · ·) for the barrier-center donor. (b) The long-dashed lines (— —) stand for the barrier-edge donor and the short-dashed lines (– – – –) for the outer-well-edge donor.

L_b increases and the wave function in the double-width well begins to separate into single-well wave functions. The well-center donor is in a favorable position to have a greater probability of finding the electron in its vicinity; its binding energy quickly recovers the single-well limit. Again, only inclusion of subband mixing allows one to correctly describe the realistic situation. The outer-well-edge donor always benefits from evolution of the DQW wave function into the single-well wave function. Its binding energy monotonically increases with increasing L_b, and eventually flattens out as the average electron-donor distance becomes a constant for a fixed well size.

In Fig. 8, we display the binding energies of the $2p_-$ state as a function of L_b. The $2p_-$ donor state, due to compression of its large natural wave-function spread in the DQW structure, behaves quite differently with increasing barrier thickness L_b. All donor locations start out with roughly the same binding energies, because the highly spread out electron wave function is not sensitive to the donor location in the DQW of $L_b \approx 0$. The barrier-center donor binding energy monotonically decreases as L_b increases, for the same reason as in the case of the $1s$ state. In contrast to their $1s$ counterparts, donors outside the barrier first see their binding energies decrease with increasing barrier thicknesses. The reason is as follows. The $2p_-$-state wave function is highly compressed in the DQW of total width $2L_w + L_b$ (100 Å$+L_b$ here), so the wave function will first expand to occupy the extra space provided by the increasing L_b, thereby reducing the probability of finding the electron in the vicinity of the donor; and the binding energies will first decrease. After this initial expansion stage, the DQW wave function begins to pile up around the donor and gradually becomes effectively a single-well wave function, and the binding energies then quickly approach the single-well limit. As expected, extra confinement by the magnetic field compresses the wave function in the structure or around a donor, and therefore increases binding energies and increases the pace at which the binding energies change with increasing barrier thickness.

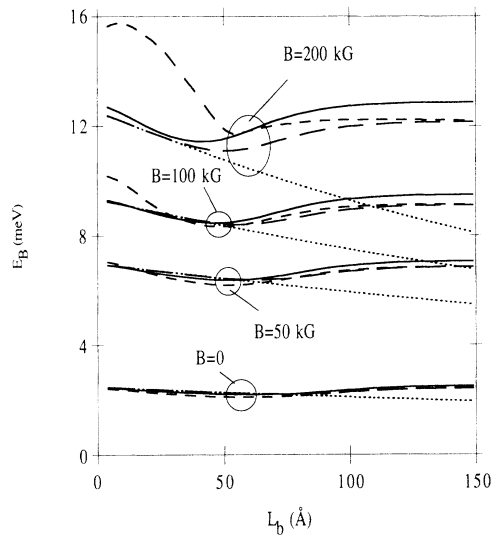

FIG. 8. The binding energy of the $2p_-$ donor state E_B as a function of barrier thickness L_b, for a fixed well size $L_w = 50$ Å, for several values of magnetic field B (kG). The solid lines (——) stand for the well-center donor, the dotted lines (· · · ·) for the barrier-center donor, the long-dashed lines (— —) for the barrier-edge donor, and the short-dahsed lines (– – – –) for the outer-well-edge donor.

IV. SUMMARY AND CONCLUSIONS

In summary, we have developed a formalism to calculate the binding energies of excitons and donors in a symmetric double quantum well in the presence of a magnetic field applied parallel to the growth axis. The extra quantum confinement by the magnetic field increases the binding energies. Effects of interwell (intersubband) coupling on the light-hole and heavy-hole exciton binding energies in the double quantum well are consistently included in our calculation. In the limit of thick potential barriers, the even-parity and odd-parity subband wave functions have degenerate energy levels; mixing of electron and hole subband wave functions strongly modifies the excitonic wave function and consequently lets one recover results for excitons in decoupled single quantum wells. We have shown that ignoring such subband mixing is a good approximation only for narrow wells *and* thin-barrier double quantum-well structures, and that such a single-subband approach can lead to qualitatively misleading conclusions when applied in wide wells *or* thick barrier DQW's.

The presence of the donor atom breaks the reflection symmetry along the growth axis, and leads to strong mixing of electron subband wave functions of even and odd parities. We have shown that inclusion of such mixing is crucial for a correct description of the donor binding energies in DQW structures with wide-ranging characteristics, and that a single-subband treatment would underestimate the binding energy in a symmetric double quantum well except in the thin-barrier *and* narrow-well structures. Using our formalism, we have correctly described the donor binding energies in DQW structures with L_b ranging from zero to several effective Bohr radii, and recovered the corresponding single-well limits in both extremes. Effects of quantum confinement provided by the magnetic field and the potential wells, and that of tunneling across the center potential barrier on the exciton binding energies, are discussed.

We have used the first two single electron and hole subbands in calculations of the exciton binding energies, and our results cover most cases one would encounter in experiments. While we have not included differences in the effective masses and dielectric constants across the GaAs-$Al_xGa_{1-x}As$ interfaces in our calculations, they have been shown by various authors to lead only to small increases in the binding energies, and would not alter the conclusions here. After the original manuscripts were submitted, Ranganathan *et al.* also reported their work

on the donor binding energies in double quantum wells, with the inclusion of subband mixing effects.[42] Our generalized formalism, when applied to the case of donor binding energies for the specific parameters, obtained results which are in agreement with the results of their calculation and experiment.

ACKNOWLEDGMENTS

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