

Excitons in double quantum wells

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Excitons in a double-quantum-well structure, consisting of two wells separated by a thin barrier, are studied. Binding energies and oscillator strengths of the exciton ground state are calculated as a function of the barrier width and the well width. It is shown that the barrier width and the barrier height give the significant influence on the dimensional character of excitons through the change of the distribution of the subband wave function.

I. INTRODUCTION

With recent developments in semiconductor technology, superlattices—that is, one-dimensional periodic thin-layer structures—have attracted much attention. These systems have interesting characteristics which are not seen in bulk materials in optical and electrical properties, and they have been actively researched from both fundamental and practical points of view.¹⁻⁶

Up to now, the study of the exciton states in such systems has been performed mainly for a single quantum well (SQW), where an electron and a hole are in the same layer and the coupling with neighboring wells is neglected.¹⁻⁹

In the present work we focus our attention on a double-quantum-well (DQW) structure consisting of two quantum wells separated by a thin potential barrier and study the lowest exciton state in this system from a general point of view. In the SQW system, subband and exciton states are determined by physical parameters such as well width and potential barrier height, and material parameters such as masses and dielectric constants. In the DQW system these subband and exciton states are also influenced by a barrier between two quantum wells: as the barrier width is suitably thin, a wave function has a significant amplitude in both wells, and then the coupling of the two wells occurs.¹⁰⁻¹⁷ This feature yields unique properties, such as the enhanced quantum-confined Stark effect, and then potential applications to optical devices can be actively studied.^{11,18-24}

In the following we study theoretically general properties of the binding energy and the oscillator strength of the exciton in a DQW system which have not been studied so far. In Sec. II the subband states in this system are discussed briefly. In Sec. III we calculate the energy, the binding energy and the oscillator strength of the exciton ground state as a function of the well width and the barrier width, using a finite-potential model and a variational method. In Sec. IV we summarize the results obtained in the present calculation.

II. SUBBAND STATE IN A DOUBLE QUANTUM WELL

First, let us consider a motion of a particle in a DQW structure consisting of two quantum wells with thickness L_w , separated by a thin potential barrier with thickness L_b (Fig. 1).^{10-12,25} In the effective-mass approximation the Hamiltonian for a particle is given by

$$H_z = \frac{p_z^2}{2m} + V(z). \quad (1)$$

Here the z axis is taken to be perpendicular to the well interfaces. The mass of the particle m is equal to m_w in the well region and m_{b1} (m_{b2}) in the middle (side) barrier region. The z components of the position and momentum of the particles are denoted z and p_z , respectively. The confinement potential $V(z)$ for a particle is assumed to be

$$V(z) = \begin{cases} 0, & L_b/2 < |z| < L_b/2 + L_w \\ V^{b1}, & |z| < L_b/2 \\ V^{b2}, & L_b/2 + L_w < |z| < \infty. \end{cases} \quad (2)$$

The solution of the Schrödinger equation with the Hamiltonian H_z is easily obtained. The symmetry of the system yields the even and odd wave functions with respect to the z coordinate. For the even or odd function, we obtain

$$\psi(z) = \begin{cases} De^{-\beta_2 z}, & z > L_b/2 + L_w \\ A \sin(\alpha z) + B \cos(\alpha z), & L_b/2 < z < L_b/2 + L_w \\ C(e^{\beta_1 z} \pm e^{-\beta_1 z}), & L_b/2 > |z| \\ \mp A \sin(\alpha z) \pm B \cos(\alpha z), & -L_b/2 > z > -L_b/2 - L_w \\ \pm De^{\beta_2 z}, & z < -L_b/2 - L_w \end{cases} \quad (3)$$

where $\alpha = (2m_w E_l)^{1/2} / \hbar$ and $\beta_i = [2m_{bi}(V^{bi} - E_l)]^{1/2} / \hbar$ ($i = 1$ or 2). E_l is the eigenenergy of the l th subband of a particle. By matching $\psi(z)$ and $(1/m_i)d\psi(z)/dz$ ($i = w$,

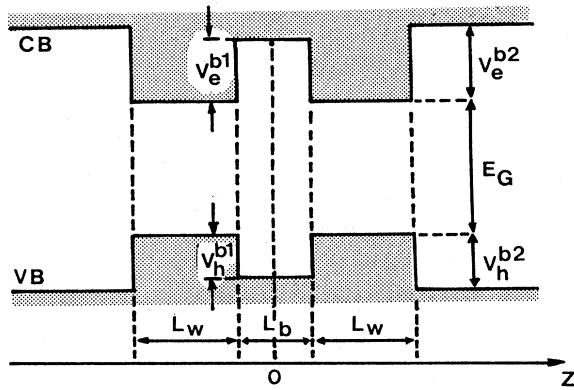


FIG. 1. Double-quantum-well profile along the z axis normal to layer interfaces. Here, CB, VB, and E_G denote the conduction- and valence-band edges, and the gap energy, respectively.

$b1$, or $b2$) at the interfaces $z = L_b/2$ and $L_b/2 + L_w$, we obtain the following equations for the l th subband eigenenergy: for the even wave function,

$$S_1[1 - S_2 \tan(\alpha L_w)] + \tanh(\beta_1 L_b/2)[S_2 + \tan(\alpha L_w)] = 0, \quad (4)$$

and for the odd wave function,

$$S_2 + \tan(\alpha L_w) + \tanh(\beta_1 L_b/2)S_1[1 - S_2 \tan(\alpha L_w)] = 0, \quad (5)$$

where $S_i = m_{bi}\alpha / (m_w\beta_i)$ ($i = 1$ or 2). If the length and energy are conveniently measured in units of the well width L_w and the first-subband energy for the SQW in the infinite-potential-barrier model $E_1^\infty = \pi^2\hbar^2 / (2m_w L_w^2)$, our system is characterized by the following five parameters: the normalized potential barrier $\bar{V}^{b1} = V^{b1} / E_1^\infty$, the barrier-well width ratio $\sigma_L = L_b / L_w$, the potential-barrier ratio $\sigma_V = V^{b2} / V^{b1}$, and the effective-mass ratio $\sigma_{mi} = m_{bi} / m_w$ ($i = 1$ and 2). Changing these physical parameters, we have calculated the normalized energy $\bar{E}_l = E_l / E_1^\infty$ and the wave function $\psi_l(z)$ for the lowest two subband states ($l = 1, 2$). Results with $\sigma_V = \sigma_{m1} = \sigma_{m2} = 1$ are shown in Figs. 2 and 3.

In Fig. 2(a) we plot the subband energy \bar{E}_l as a function of the barrier-well width ratio σ_L for three normalized potential barriers, i.e., $\bar{V}^b \equiv \bar{V}^{b1} = \bar{V}^{b2} = 1, 10$, and 100 . In the figure we see that differences between \bar{E}_1 and \bar{E}_2 become smaller for larger σ_L . This reflects the fact that the coupling of two wells becomes weak for larger σ_L . Figure 2(b) gives the subband energy \bar{E}_l as a function of the normalized potential barrier \bar{V}^b for four barrier-well width ratios, i.e., $\sigma_L = 0, 0.01, 0.10$, and 1.00 . When σ_L is zero, our system is just that of the SQW with well width $2L_w$. Thus energies $\bar{E}_1 = \frac{1}{4}$ and $\bar{E}_2 = 1$ are obtained in the infinite-barrier case ($\bar{V}^b = \infty$) and both \bar{E}_1 and \bar{E}_2 decrease monotonically for decreasing \bar{V}^b , as seen in the figure. This behavior is rather different from that

for the finite σ_L , where the coupling of the lowest state of each SQW, via the potential-barrier region, yields the lowest two states, except for the very-small- \bar{V}^b case. In this very-small- \bar{V}^b case there is only one bound state in our DQW system. We see in Fig. 2(b) that the energy differences between \bar{E}_1 and \bar{E}_2 become smaller for larger potential barrier \bar{V}^b because of the smaller coupling of the two wells.

In Fig. 3 we have plotted the square of the wave-function amplitudes, $|\psi_l(z)|^2$, of the lowest two states for three different barrier-well width ratios $\sigma_L = 0.0, 0.1$, and 1.0 with the normalized potential barrier $\bar{V}^b = 1.0$. We find in this figure that, for increasing barrier-well width

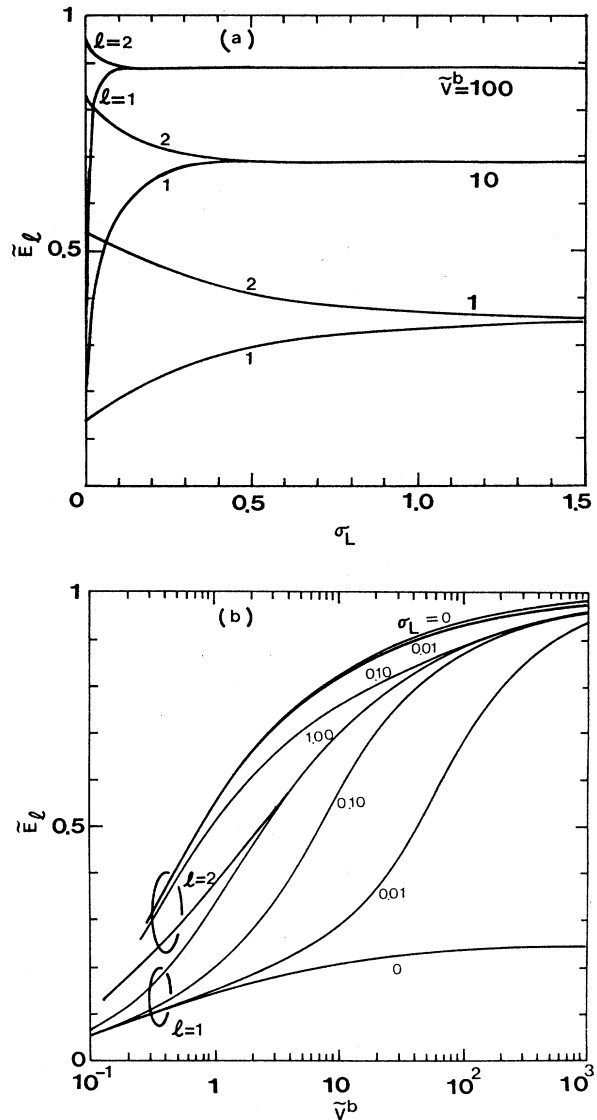


FIG. 2. (a) Normalized subband energy \bar{E}_l for $l = 1$ and 2 as a function of the barrier-well width ratio σ_L . The normalized potential barrier is taken to be $\bar{V}^b = 1, 10$, and 100 . (b) Normalized subband energy \bar{E}_l for $l = 1$ and 2 as a function of the normalized potential barrier \bar{V}^b . The barrier-well width ratio is taken to be $\sigma_L = 0, 0.01, 0.10$, and 1.00 .

σ_L , the wave-function amplitudes of the lowest state ($l=1$) at $z=0$ becomes smaller. Then the square of the wave function amplitude of the $l=1$ state becomes similar to that of the $l=2$ state. This reflects the smaller coupling of two wells for larger σ_L .

Here we briefly discuss the dependence of the subband states on σ_V and $\sigma_m \equiv \sigma_{m1} = \sigma_{m2}$ with the fixed values $\bar{V}^{b1} = 1.0$ and $\sigma_L = 0.1$. Setting $\sigma_m = 1$, we increase σ_V , and then the subband energy \bar{E}_l ($l=1,2$) becomes larger than that of Fig. 2(b): for example, $\bar{E}_1 = 0.22$ and $\bar{E}_2 = 0.60$ for $\sigma_V = 2$, which are compared to $\bar{E}_1 = 0.20$ and $\bar{E}_2 = 0.51$ for $\sigma_V = 1$. This is because for larger σ_V the penetration of the particle into the outside barriers is suppressed and the confinement effect becomes stronger. Next, we set $\sigma_V = 1$ and increase σ_m . Then, the subband energy \bar{E}_l ($l=1,2$) becomes smaller than that in Fig. 2(b): for example, $\bar{E}_1 = 0.17$ and $\bar{E}_2 = 0.43$ for $\sigma_m = 2$ and $\bar{E}_1 = 0.20$ and $\bar{E}_2 = 0.51$ for $\sigma_m = 1$. This smaller sub-

band energy is due to the fact that the kinetic-energy term of the particle in the barrier region decreases as the mass $m_b = m_{b1} = m_{b2}$ increases.

III. EXCITON STATE IN A DOUBLE QUANTUM WELL

Next, we discuss excitons in the DQW. Here we confine ourselves to the case that materials of the middle and side barrier parts are the same. The Hamiltonian of the system is written as

$$H = H_{ze} + H_{zh} + \frac{p_x^2 + p_y^2}{2\mu} - \frac{e^2}{\epsilon r}. \quad (6)$$

Here we have assumed the isotropic band for an electron (with mass m_e) and the ellipsoidal band for a hole (with mass m_h in the x - y plane and m_{hz} in the z direction). The kinetic-energy part of the center-of-mass motion of an electron and a hole in the layer plane is omitted from the Hamiltonian since x and y components of the momentum, P_x and P_y , being conjugate to center of mass coordinates X and Y , are constants of motion. H_{ze} (H_{zh}) is given by H_z of Eq. (1) with the replacement of mass m and barrier-potential heights $V^b \equiv V^{b1} = V^{b2}$ by electron mass m_e (hole mass m_{hz}) and potential heights $V_e^b \equiv V_e^{b1} = V_e^{b2}$ ($V_h^b \equiv V_h^{b1} = V_h^{b2}$), respectively. The third term on the right-hand side of Eq. (6) represents the kinetic-energy part of the relative motion with position $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_h$, momentum $\mathbf{p} = -i\hbar\partial/\partial\mathbf{r}$, and mass $\mu = m_e m_h / (m_e + m_h)$ in the x - y plane. The Coulomb attraction between the electron and hole is described by the last term of Eq. (6), where ϵ is the background dielectric constant. We use a variational method to calculate the exciton state.²⁻⁴ The following variational wave function for the $1s$ -type state, associated with the l_e th electron and l_h th hole subbands, is chosen as

$$\Phi^{(l_e, l_h)} = N^{(l_e, l_h)} \psi_{l_e}(z_e) \psi_{l_h}(z_h) \phi(r). \quad (7)$$

Here, $N^{(l_e, l_h)}$ is the normalized factor. The normalized l_e th electron (l_h th hole) subband wave function $\psi_{l_e}(z_e)$ [$\psi_{l_h}(z_h)$] is calculated as in Sec. II. $\phi(r)$ describes the relative motion and is chosen to be of the form

$$\phi(r) = \exp\{-[\alpha^2(x^2 + y^2) + \beta^2 z^2]^{1/2}\}, \quad (8)$$

where α and β are variational parameters. The exciton energy can be calculated from

$$E^{(l_e, l_h)} = \min_{(\alpha, \beta)} \langle \Phi^{(l_e, l_h)} | H | \Phi^{(l_e, l_h)} \rangle, \quad (9)$$

and the binding energy is determined by

$$E^{B(l_e, l_h)} = E_{l_e}^e + E_{l_h}^h - E^{(l_e, l_h)}. \quad (10)$$

Here, $E_{l_e}^e$ ($E_{l_h}^h$) is the l_e th electron (l_h th hole) subband energy. Also, the optical oscillator strength can be obtained from^{4-6,26}

$$f^{(l_e, l_h)} = B_b |\phi(0) F(0) N^{(l_e, l_h)}|^2 / 2L_w. \quad (11)$$

Here, B_b is proportional to $|M_{cv}|^2$, where M_{cv} is the optical transition matrix element between the conduction and

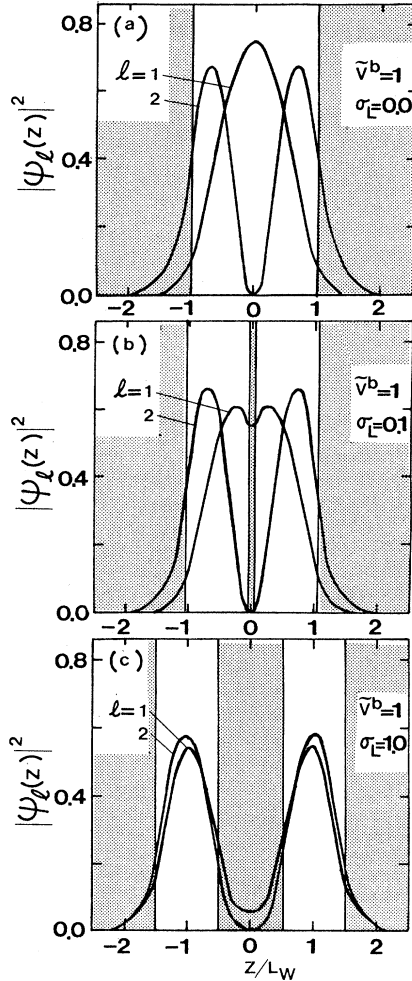


FIG. 3. Square of the wave-function amplitude, $|\psi_l(z)|^2$, for the lowest two subband states ($l=1,2$) as a function of the normalized position z/L_w with the normalized potential barrier $\bar{V}^b=1.0$. (a), (b), and (c) correspond to the barrier-well widths $\sigma_L=0.0, 0.1$, and 1.0 , respectively.

valence bands. The electron-hole-overlap function $F(0)$ is given by

$$F(0) = \int_{-\infty}^{+\infty} dz \psi_{l_e}(z) \psi_{l_h}(z). \quad (12)$$

In the following, all energies are expressed in terms of the Rydberg R ($=\mu e^4/2\epsilon^2\hbar^2$) and all lengths in terms of the Bohr radius a_B ($=\epsilon\hbar^2/\mu e^2$). If we neglect the difference in masses for the well and barrier parts, the present system is characterized by the following six parameters: the well width L_w , the barrier-well width ratio $\sigma_L = L_b/L_w$, the total potential barrier $V_T^b = V_e^b + V_h^b$, the band offset $Q_e = V_e^h/V_T^b$, the electron-hole mass ratio $\sigma_m^{eh} = m_e/m_h$, and the anisotropic hole mass ratio $\sigma_m^{hz} = m_{hz}/m_h$. In the present model calculation we choose $\sigma_m^{eh} = 1.0$, $\sigma_m^{hz} = 5.0$, $Q_e = 0.6$, and $V_T^b = 120R$, whose values roughly correspond to the GaAs well and the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ($x = 0.3$) barrier.

In Fig. 4 the exciton energy $E^{(l_e, l_h)}$ and the binding energy $E^{B(1,1)}$ of the lowest exciton state are shown as a function of the well width L_w . We see in Fig. 4(a) that the exciton energy $E^{(l_e, l_h)}$ decreases monotonically as L_w becomes larger: this behavior is the same as that of the interband transition energy from the l_h th hole subband to the l_e th electron subband. Figure 4(b) gives the binding energy $E^{B(1,1)}$ for three different barrier widths, namely $L_b = 0.05a_B$, $0.10a_B$, and $1.00a_B$. In the figure we also plot $E^{B(1,1)}$ in the cases of $L_b = 0a_B$ and $L_b = \infty a_B$, which correspond to the SQW with the well widths $2L_w$ and L_w , respectively. We find that for a given finite-potential-barrier value the binding energy has the maximum in the range $0 < L_w < 0.2a_B$. The reason for the occurrence of a maximum is the same as that in the SQW.³ When the well width L_w decreases from large values, an exciton is confined in the well and the two-dimensional character appears in the large binding energy. However, for the further decrease of L_w , the penetration of the exciton wave function into barrier parts becomes large and then two-dimensional character of exciton starts to decrease, while three-dimensional character increases.³ This explains why the maximum of $E^{B(1,1)}$ appears. We note that in the infinite-potential-barrier case ($V_e^b = V_h^b = \infty R$) this penetration of the wave function does not occur and the purely two-dimensional result of the binding energy, $4R$, is obtained for $L_w = 0a_B$ as in the case of the SQW.²⁻⁴ If we consider the thick-barrier case (the large- L_b case), we expect the weak coupling of the wells. Thus, as seen in Fig. 4(b), the exciton binding energy becomes close to that of the SQW with the well width L_w .

In Fig. 5 we show the exciton energy $E^{(l_e, l_h)}$ and the binding energy of the exciton, $E^{B(1,1)}$, as a function of the barrier width L_b . Figure 5(a) shows how the coupling of the two wells affects the exciton energy: for larger L_b all exciton energies— $E^{(l_e, l_h)}$ s—are close because of the smaller coupling of the wells. In Fig. 5(b) the binding energies $E^{B(1,1)}$ are shown for three different values of well widths, namely $L_w = 0.1a_B$, $0.2a_B$, and $0.6a_B$. We find that for a given value of L_w the exciton binding energy $E^{B(1,1)}$ has a minimum. The value of L_b at the minimum

is smaller for larger L_w . The reason for such a behavior is as follows. We know that the binding energy of the DQW in the thick limit $L_b = \infty$ (in the thin limit $L_b = 0$) is that of the SQW with the well width L_w ($2L_w$). When L_b is large enough, the binding energy keeps that of the SQW with the well width L_w to some extent, since the wave function rarely goes into the other well. As L_b is reduced, $E^{B(1,1)}$ decreases due to the spreading of the wave function into both wells and to the smaller electron-hole Coulomb interaction. Next, we consider another case, i.e., the small- L_b case. When L_b increases

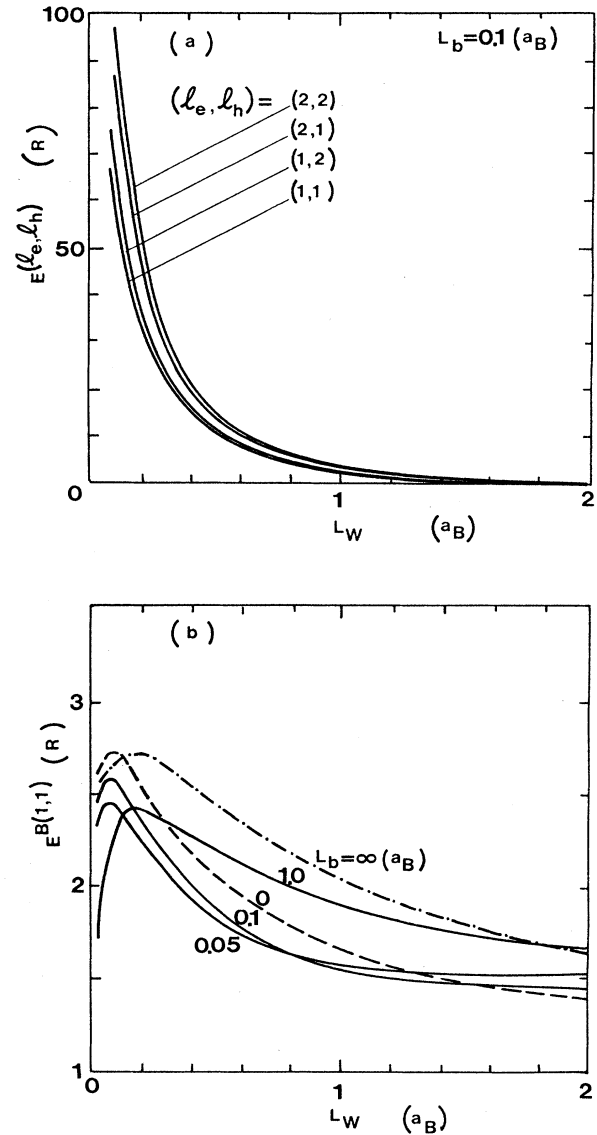


FIG. 4. (a) Exciton energy $E^{(l_e, l_h)}$ as a function of the well width L_w for the barrier width $L_b = 0.1a_B$. (b) Binding energy of the lowest exciton state, $E^{B(1,1)}$, as a function of the well width L_w for three different barrier widths, namely $L_b = 0.05a_B$, $0.1a_B$, and $1.0a_B$. The dashed and dashed-dotted lines show the binding energy in the cases $L_b = 0a_B$ and ∞a_B , respectively.

from zero, the electron and hole subband wave functions have dips at $z_e = z_h = 0$ in the middle barrier part. This yields the smaller electron-hole Coulomb interaction, resulting in the smaller exciton binding energy. Thus, the minimum of the binding energy as a function of L_b originates from the change of the distribution of the wave function due to the quantum-size effect.

In Fig. 6 the oscillator strength $f^{(1,1)}$ is plotted as a function of the barrier width L_b for three different values of L_w , i.e., $L_w = 0.1a_B$, $0.2a_B$ and $0.6a_B$. We see in the figure that a minimum of $f^{(1,1)}$ appears for each value L_w . The reason for the appearance of the minimum is the same as that of $E^{B(1,1)}$ in Fig. 5(b).

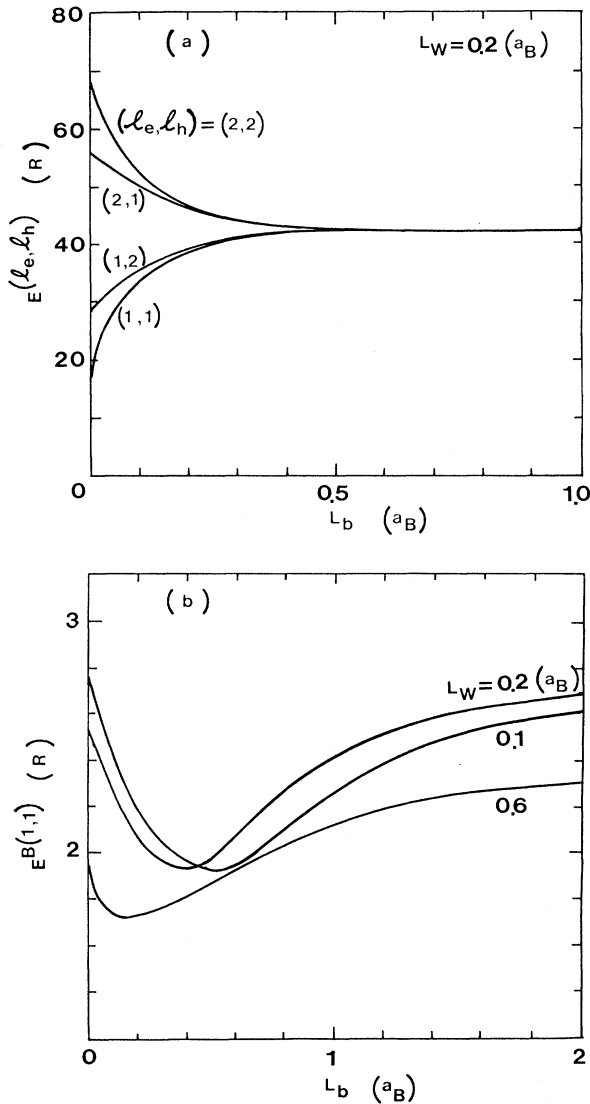


FIG. 5. (a) Exciton energy $E^{(l_e, l_h)}$ as a function of the barrier width L_b for the well width $L_w = 0.2a_B$. (b) Binding energy of the lowest exciton state, $E^{B(1,1)}$, as a function of the barrier width L_b . The well width is taken to be $L_w = 0.1a_B$, $0.2a_B$, and $0.6a_B$.

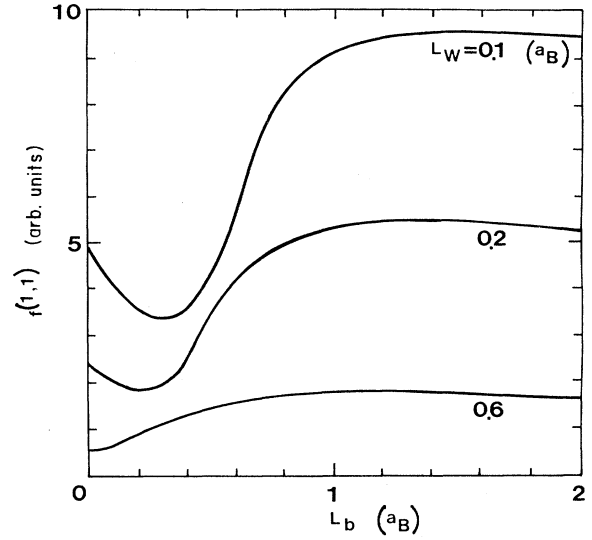


FIG. 6. Oscillator strength of the lowest exciton state, $f^{(1,1)}$, as a function of the well width L_b . The well width is taken to be $L_w = 0.1a_B$, $0.2a_B$, and $0.6a_B$.

Here we discuss the effects of the potential-barrier height on excitons. In addition to the case of the total potential barrier $V_T^b = 120R$, we have also calculated exciton states for the case of $V_T^b = 60R$ and $240R$. When $L_w = L_b = 0.2a_B$, the obtained values of $E^{B(1,1)}$ are $2.02R$ and $2.11R$ for $V_T^b = 60R$ and $240R$, respectively. These are compared with $2.07R$ for $V_T^b = 120R$. From these results we can say that for fixed L_w and L_b the larger the barrier potential height V_T^b , the larger the value of $E^{B(1,1)}$, though the differences are small.

So far, we have assumed that excitons are associated with each electron and hole subband state. When the energy difference between the first and second subband state is small, it may be necessary to consider intersubband coupling of the excitons. To examine this effect, we have calculated excitons associated with the subband $l_e, l_h = 1, 2$, and have then considered the coupling of these excitons: a linear combination of states $\Phi^{(l_e, l_h)}$ ($l_e, l_h = 1, 2$) is used,

$$\Psi = \sum_{l_e, l_h=1}^2 A(l_e, l_h) \Phi^{(l_e, l_h)}. \quad (13)$$

Thus, the exciton energy with the coupling E_c is calculated from

$$\det |M(l_e, l_h, l'_e, l'_h)| = 0 \quad (l_e, l_h, l'_e, l'_h = 1, 2). \quad (14)$$

Here,

$$M(l_e, l_h, l'_e, l'_h) = \langle \Phi^{(l_e, l_h)} | H | \Phi^{(l'_e, l'_h)} \rangle - E_c \langle \Phi^{(l_e, l_h)} | \Phi^{(l'_e, l'_h)} \rangle.$$

Equation (14) is a 4×4 determinant, but this equation is reduced into two 2×2 determinants, because of the symmetry properties of the wave function with respect to the z_e and z_h coordinates. Then the lowest exciton energy is obtained from the following 2×2 determinant, i.e.,

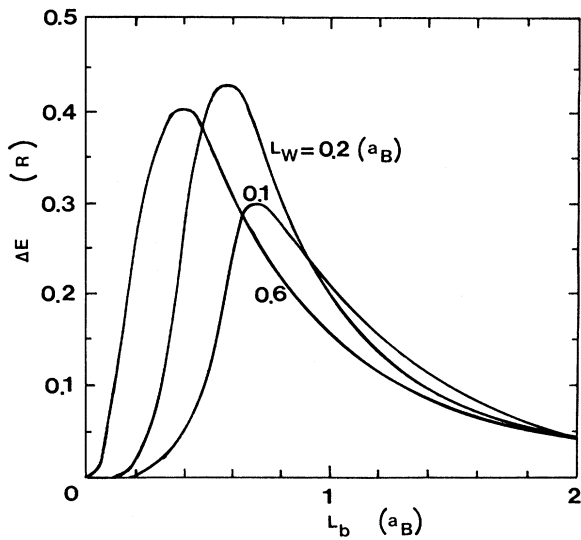


FIG. 7. Change of the exciton energy due to intersubband coupling, ΔE , as a function of the barrier width L_b . The well width is taken to be $L_w = 0.1a_B, 0.2a_B$, and $0.6a_B$.

$$\begin{vmatrix} M(11,11) & M(11,22) \\ M(22,11) & M(22,22) \end{vmatrix} = 0. \quad (15)$$

Then the binding energy of the lowest exciton, E_c^B , is given by

$$E_c^B = E_1^e + E_1^h - E_c. \quad (16)$$

Also, the oscillator strength with the coupling f^c can be calculated from

$$f^c = B_b \left| \sum_{l_e, l_h=1}^2 A(l_e, l_h) N^{(l_e, l_h)} F(0) \right|^2. \quad (17)$$

According to Eqs. (15)–(17), we have performed a numerical calculation of the exciton energy E_c , the exciton binding energy E_c^B , and the oscillator strength f^c : results obtained are similar to those in Figs. 4–6. The change of the exciton energy due to the intersubband coupling $\Delta E \equiv E_c - E^{(1,1)} = E_c^B - E^{B(1,1)}$ is shown in Fig. 7. It can

be seen that ΔE depends very much on the barrier width L_b . Comparison of the results in Figs. 5 and 7 shows that the intersubband coupling of the excitons yields the larger binding energy by at most 20%. The decrease of ΔE for large L_b is due to a decrease of the coupling of wells. Also, we find that for the change of L_b the oscillator strength f^c behaves similar to $f^{(1,1)}$ in Fig. 6. Changes of the oscillator strengths due to the intersubband coupling are not so large: for example, when L_w is $0.1a_B$, $f^c = 4.30$ and 4.42 and $f^{(1,1)} = 4.31$ and 3.68 in the same units as Fig. 6 are obtained at the values of $L_b = 0.1a_B$ and $0.4a_B$, respectively. The above results indicate that the qualitative behavior of excitons in the DQW system is described without the intersubband coupling, but the coupling needs to be considered for the quantitative discussion in the region of the barrier width $0.2a_B \lesssim L_b \lesssim 0.8a_B$.

IV. SUMMARY

We have studied the lowest exciton state in the double-quantum-well structure consisting of two wells separated by a thin barrier. The variational calculation has shown that the exciton binding energy and the oscillator strength are strongly affected by a barrier width L_b : both exciton binding energy and oscillator strength have a minimum as a function of L_b . This reflects the distribution of the subband wave function in the double-quantum-well system which affects the magnitude of the electron-hole Coulomb interaction. The above results show how the dimensional character of excitons, such as two- or three-dimensional character, appears in the double-quantum-well system. Also, it is shown that the intersubband coupling of excitons needs to be considered for the quantitative discussion generally, though this does not affect the qualitative behavior of excitons.

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