

Subbands and excitons in a quantum well in an electric field

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The effects of an electric field on the subbands and excitons in a quantum well are discussed with the use of an infinite-potential-barrier model. It is shown that for increasing electric fields the energy of the lowest subband state becomes lower, while that of higher subband states becomes slightly higher initially and then decreases. This behavior of the subbands affects excitonic properties for which a model variational calculation of the energy and the oscillator strength is performed. It is found that (1) the exciton energy shift depends strongly on the electron and hole subbands with which the excitons are associated and that (2) for large electric fields, oscillator strengths for usually forbidden excitons with different electron and hole subband indices become similar in magnitude to those for allowed excitons. These results agree well with the main features of optical absorption experiments.

I. INTRODUCTION

The effects of electric fields on the optical properties of quantum well (QW) are attracting much attention.¹⁻¹¹ In the optical properties of QW systems, excitons yield strong peaks in the spectra and play an important role. For absorption spectra in electric fields, we find that (1) exciton resonance remains resolved even for very high fields (~ 50 times the classical ionization field),² (2) the forbidden transition in zero field can be observed with large electric fields^{3,9} and (3) the exciton energy shift is very different between the lowest subband excitons and higher subband excitons.^{3,9} In luminescence spectra, a lifetime enhancement for excitons is observed for larger electric fields,^{7,10} although some experiments show a decrease.^{6,11}

As yet, discussion has been focused mainly on the lowest subband excitons. In the present work we pay attention to exciton states with higher subbands and perform a model variational calculation, based on the infinite-potential-barrier model (IPBM), in order to discuss the main features of experimental results for excitons with various electron and hole subband indices. In the following, we discuss subband states in the presence of an electric field and then calculate and discuss excitonic properties.

II. SUBBAND STATES IN AN INFINITE QUANTUM WELL IN AN ELECTRIC FIELD

We consider a particle, with charge e (> 0) and mass m_z , in a quantum well under an electric field F . The field F is applied in the z direction, i.e., perpendicular to the material layers. The Schrödinger equation of the system is given by

$$H_z \psi(z) = (H_{z0} - eFz) \psi(z) = E \psi(z), \quad (1)$$

where the Hamiltonian without an electric field, H_{z0} , is written as

$$H_{z0} = \frac{p_z^2}{2m_z} + V_{\text{conf}}(z). \quad (2)$$

Here z and p_z are the z components of the position and the momentum of the particle, respectively. For the IPBM the confinement potential $V_{\text{conf}}(z)$ is zero for $|z| < L/2$ and infinite for $|z| > L/2$, where L is the well width. The Hamiltonian H_{z0} has an eigenenergy $E_l^{(0)} = (\pi \hbar l)^2 / (2m_z L^2)$ and the corresponding wave function $\psi_l^{(0)}(z) = \sqrt{2/L} \cos(\pi lz/L - \alpha_l)$, where l ($= 1, 2, \dots$) is a subband index and $\alpha_l = 0$ ($\pi/2$) for odd (even) values of l .

We look for the solution of Eq. (1) in a similar way as in Ref. 2 with the use of the Airy functions $\text{Ai}(x)$ and $\text{Bi}(x)$. Introducing the new variable

$$Z = - \left[\frac{2m_z}{(e \hbar F)^2} \right]^{1/3} (E + eFz), \quad (3)$$

Eq. (1) for $|z| < L/2$ is converted to the new equation,

$$\frac{d^2 \tilde{\psi}(Z)}{dZ^2} - Z \tilde{\psi}(Z) = 0. \quad (4)$$

Then, the wave function of the l th solution of Eq. (1) is written as

$$\psi_l(z) \equiv \tilde{\psi}_l(Z_l) = c_{1l} \text{Ai}(Z_l) + c_{2l} \text{Bi}(Z_l), \quad (5)$$

where Z_l is given by the right-hand side of Eq. (3) with $E = E_l$, which is the l th eigenenergy. The boundary condition $\psi_l(-L/2) = \psi_l(L/2) = 0$ determines the coefficients c_{il} of the wave function $\psi_l(z)$ and the eigenenergy E_l : the energy E_l is the l th solution of the following equation:

$$S(E_l) \equiv \text{Ai}(Z_l^+) \text{Bi}(Z_l^-) - \text{Ai}(Z_l^-) \text{Bi}(Z_l^+) = 0, \quad (6)$$

where Z_l^+ (Z_l^-) is given by the right-hand side of Eq. (3) with $E=E_l$ and $z=L/2$ ($-L/2$). It should be noted that, as shown in Ref. 2, using the normalized energy $\bar{E}_l=E_l/E_1^{(0)}$ and the normalized field strength $\bar{F}=eFL/E_1^{(0)}$ allows Eq. (6) to be expressed by only two quantities, \bar{E}_l and \bar{F} through the equation $Z_l^\pm = -(\pi/\bar{F})^{2/3}(\bar{E}_l \pm \bar{F}/2)$. This means that the solution of Eq. (6) is universal and can be used for both electrons and holes with the replacement of $E_1^{(0)}$ by the corresponding values.

We have solved Eq. (6) numerically. The results obtained for the energies of the first three states $l=1-3$ are plotted in Fig. 1. It is readily seen that the shift of the subband energy due to electric fields is very different between the lowest $l=1$ state and the higher $l=2$ or 3 state. For increasing electric fields, the $l=1$ state shows a large negative energy shift, while higher $l \geq 2$ states have a small positive shift for smaller electric fields and a negative shift for very large electric fields. This very different behavior of the energy shift between the lowest state and higher states reflects the change in the wave function under electric fields. In Fig. 2 we have plotted the wave function of the first three states for three different electric fields ($\bar{F}=0, 20$, and 50). We see in Fig. 2 that for stronger electric fields the wave function of the lowest $l=1$ state has a larger amplitude in the positive region of

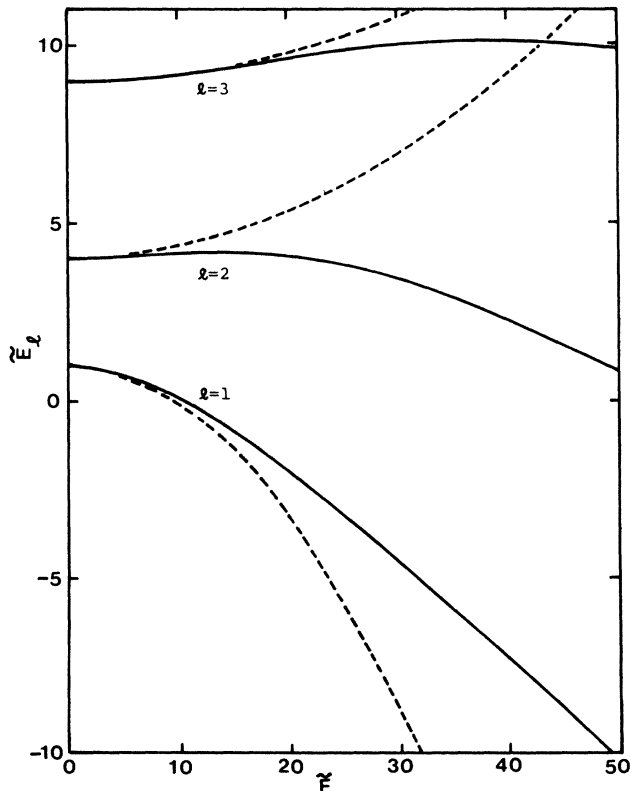


FIG. 1. Normalized subband energy $\bar{E}_l \equiv E_l/E_1^{(0)}$ for $l=1, 2$, and 3 versus normalized electric field $\bar{F} \equiv eFL/E_1^{(0)}$. The solid and dashed lines show the exact and second-order energy shifts, respectively.

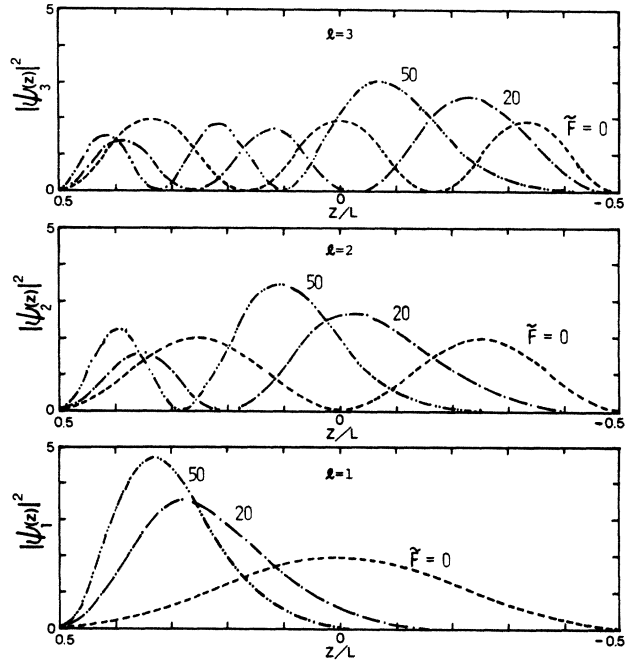


FIG. 2. Amplitude of the normalized subband wave function $|\psi_l(z)|^2$ for $l=1, 2$, and 3 versus the normalized position z/L . The normalized electric field is taken to be $\bar{F}=0, 20$, and 50.

z , reflecting the attractive force in the z direction. On the other hand, although for higher subband states the wave functions move to the z direction as a whole, they still have a large amplitude in the $z < 0$ region even for large \bar{F} such as $\bar{F} \sim 20$. This yields a positive energy shift for $l \geq 2$ states.

In Fig. 1 we have also plotted the subband energy, which is obtained from the second-order energy shift,^{12,13}

$$\begin{aligned} \Delta E_l^{(2)} &= \sum_{m \neq l} \frac{|\langle \psi_m | eFz | \psi_l \rangle|^2}{E_l^{(0)} - E_m^{(0)}} = C_l \frac{m_z e^2 F^2 L^4}{\hbar^2} \\ &= C_l \frac{\pi^2}{2} \bar{F}^2 E_1^{(0)}, \end{aligned} \quad (7)$$

where $C_l = (l^2 \pi^2 - 15)/(24l^4 \pi^4)$. It should be noted that C_1 is negative, while C_l 's for $l \geq 2$ are positive (numerically $C_1 \approx -2.1945 \times 10^{-3}$, $C_2 \approx 6.5441 \times 10^{-4}$, and $C_3 \approx 3.8987 \times 10^{-4}$). As seen in Fig. 1 the second-order energy shift can describe the exact energy shift for smaller \bar{F} rather well. In passing we note that the variational method of Bastard *et al.*,¹ which uses the simple variational wave function $\psi \propto \cos(\pi z/L) \exp(-\beta z/L)$, yields the similar result as the exact one for the $l=1$ subband energy as shown in Ref. 2.¹⁴

III. EXCITONS IN A QUANTUM WELL IN AN ELECTRIC FIELD

Now we discuss excitons in the presence of an electric field. If we treat the degenerate valence bands as ellipsoidal heavy- and light-hole bands,¹⁵ the Hamiltonian of the system is written as

$$H = H_{ez} + H_{hz} + \frac{P_x^2 + P_y^2}{2M} + \frac{p_x^2 + p_y^2}{2\mu} - \frac{e^2}{\epsilon r}. \quad (8)$$

Here H_{ez} (H_{hz}) is given by H_z of Eq. (1) with the replacement of mass m_z and charge e by electron mass m_e (hole mass m_{hz}) and charge $-e$ (e). The third and fourth terms of the right-hand side of Eq. (8) represent, respectively, the kinetic operators of the center of mass motion (mass $M = m_e + m_h$) and the relative motion [mass $\mu = (m_e^{-1} + m_h^{-1})^{-1}$] of an exciton in the x - y plane, being parallel to the material layers. For the heavy-hole (hh) exciton the hole mass m_h in the x - y plane and m_{hz} in the z direction are given by $m_h = (\gamma_1 + \gamma_2)^{-1} m_0$ and $m_{hz} = (\gamma_1 - 2\gamma_2)^{-1} m_0$, respectively. Here γ_i 's are Luttinger parameters¹⁶ and m_0 is the free electron mass. The electron-hole Coulomb interaction is described by the last term of Eq. (8), where $\mathbf{r} = (x, y, z)$ is the electron-hole relative distance and ϵ is the dielectric constant of the medium.

We use a variational method to calculate exciton states.^{2,4,15,17,18} The following variational wave function is chosen for the $1s$ -type state, associated with the l_e th electron and l_h th hole subbands,

$$\Phi = N_{1s} \psi_{l_e}(z_e) \psi_{l_h}(z_h) \phi_{1s}(\mathbf{r}). \quad (9)$$

Here we have dropped the center-of-mass motion in the x - y plane. The normalized factor is denoted by N_{1s} . $\psi_{l_e}(z_e)$ [$\psi_{l_h}(z_h)$] is the normalized l_e th electron (l_h th hole) subband wave function which can be obtained from the procedure in Sec. II. $\phi_{1s}(\mathbf{r})$ is given by

$$\phi_{1s}(\mathbf{r}) = \exp\{-[\alpha_{1s}^2(x^2 + y^2) + \beta_{1s}^2 z^2]^{1/2}\}, \quad (10)$$

where α_{1s} and β_{1s} are variational parameters. Then, as the energy of an exciton is given by

$$E_{1s}^{(l_e, l_h)} = \min_{(\alpha_{1s}, \beta_{1s})} \langle \Phi | H | \Phi \rangle, \quad (11)$$

the energy shift of an exciton due to the electric field is calculated from

$$\Delta E_{1s}^{(l_e, l_h)} = E_{1s}^{(l_e, l_h)} - (E_{1s}^{(l_e, l_h)})_{F=0} \quad (12)$$

and the binding energy is obtained from

$$E_{1s}^{B(l_e, l_h)} = E_{l_e}^{(e)} + E_{l_h}^{(h)} - E_{1s}^{(l_e, l_h)}, \quad (13)$$

where $E_{l_e}^{(e)}$ ($E_{l_h}^{(h)}$) is the l_e th electron (l_h th hole) subband energy. Also the oscillator strength per unit volume is given by^{8,18}

$$f_{1s}^{(l_e, l_h)} = B_b |\phi_{1s}(0)|^2 (N_{1s}^2 / L) F(0), \quad (14)$$

where $B_b = 2 |M_{cv}|^2 / m_0 \hbar \omega$. Here M_{cv} is the optical transition matrix element between the conduction and valence bands and $\hbar \omega$ is the photon energy. The electron-hole overlap function $F(0)$ is given by

$$F(0) = \left| \int_{-L/2}^{L/2} dz \phi_{l_e}(z) \phi_{l_h}(z) \right|^2. \quad (15)$$

Here we discuss rough criteria on the validity of the present IPBM calculation. We consider an electron (a

hole) with the finite potential barrier V_e^0 (V_h^0). The effect of the finite potential is important, unless the most of the amplitude of an electron (a hole) is inside the well. This yields the condition for the IPBM; for electron $(\pi \hbar l_e)^2 / 2m_e L^2 < V_e^0 - eFL/2$, which can be rewritten as $L_e \equiv l_e \pi a_B [\mu \mathcal{R}_y / m_e (V_e^0 - eFL/2)]^{1/2} < L$. Here a_B ($= \epsilon \hbar^2 / \mu e^2$) and \mathcal{R}_y ($= \mu e^4 / 2\epsilon^2 \hbar^2$) denote the Bohr radius and Rydberg energy of an exciton, respectively. Similar consideration for the hole yields the condition $L_h \equiv l_h \pi a_B [\mu \mathcal{R}_y / m_{hz} (V_h^0 - eFL/2)]^{1/2} < L$. Also we have assumed that the electron and hole subband indices are good quantum numbers for excitons. This is valid when $\mathcal{R}_y < (\pi^2 \hbar^2 / 2\mu L^2) [l^2 - (l-1)^2]$ for $l = l_e = l_h \geq 2$, which can be rewritten as $L < \pi \sqrt{2l-1} a_B$.¹⁸ These are rough criteria for the validity of the IPBM. In passing we remark that the IPBM may simulate the finite potential barrier model (FPBM), to a certain degree, by adjusting the well width. Miller *et al.*² found that by the use of the

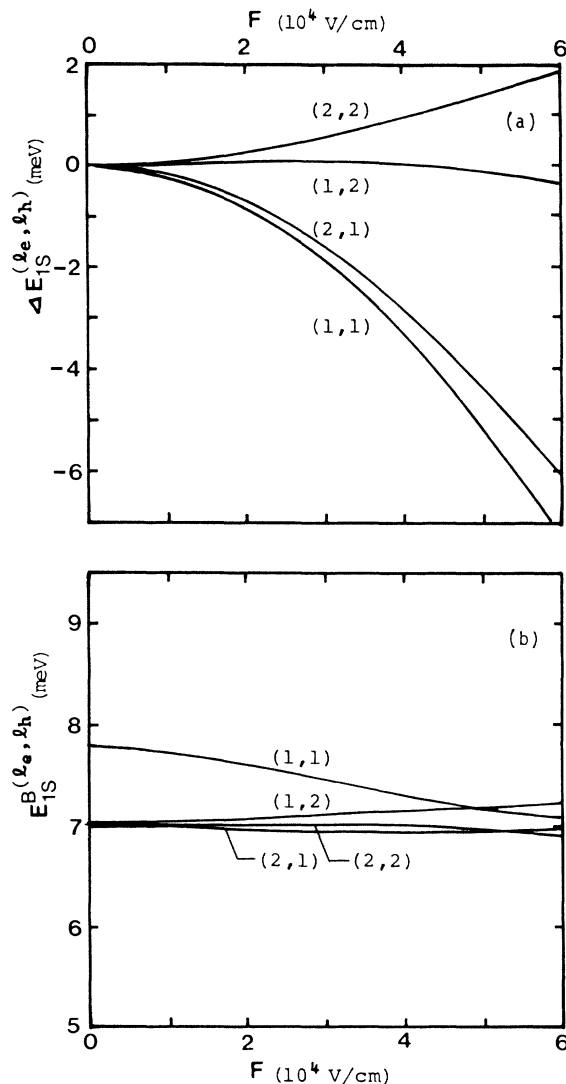


FIG. 3. (a) Energy shift $\Delta E_{1s}^{(l_e, l_h)}$ and (b) binding energy $E_{1s}^{B(l_e, l_h)}$ of excitons, associated with the l_e th electron and l_h th hole subbands versus the electric field F .

effective well width L_{eff} , which is adjusted to yield correct zero-field energies, good results for energy shifts for the lowest subband exciton under electric fields can be obtained. We have performed a numerical calculation for the hh exciton in GaAs with the well width $L = 120 \text{ \AA}$. Physical parameters are $m_e/m_0 = 0.067$, $\gamma_1 = 7.65$, $\gamma_2 = 2.41$ ($m_h/m_0 = 0.099$, $m_{hz}/m_0 = 0.353$),¹⁵ and $\epsilon_0 = 12.9$. Calculated results for excitons with $(l_e, l_h) = (1,1)$, $(1,2)$, $(2,1)$, and $(2,2)$ are shown in Figs. 3 and 4.

Now we discuss the results in Figs. 3 and 4 with experimental results. It should be noted that our comparison with the experiments is in a qualitative or semiquantitative nature because the finite potential barrier may affect the result in the experiments done so far. Figure 3(a) represents energy shifts of a $1s$ exciton $\Delta E_{1s}^{(l_e, l_h)}$ due to electric fields. The figure clearly shows the strong subband dependence of energy shifts. As seen in Eqs. (12) and (13), energy shifts of excitons arise from energy shifts of the electron and hole subbands, $\Delta E_e^{(l_e)}$ and $\Delta E_h^{(l_h)}$, in

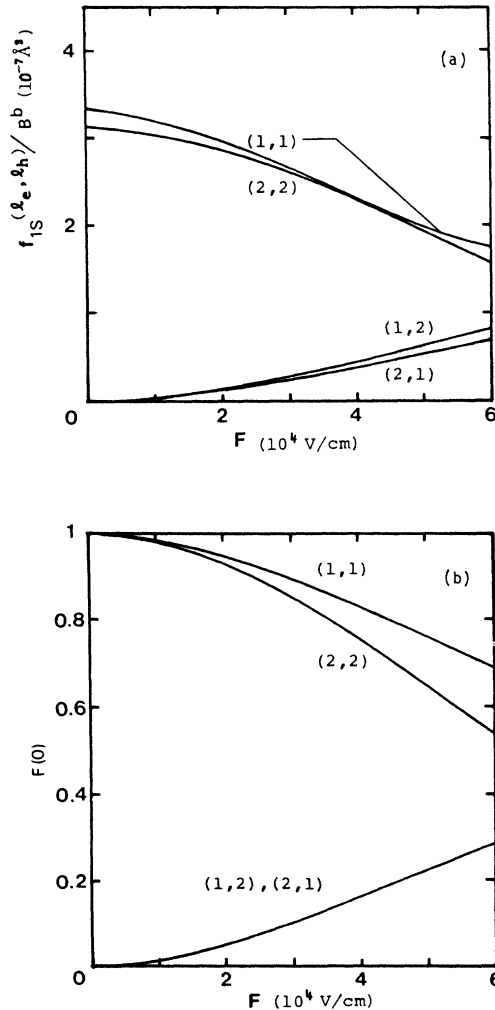


FIG. 4. (a) Oscillator strength of excitons $f_{1s}^{(l_e, l_h)}$ and (b) electron-hole overlap function $F(0)$ versus the electric field F .

addition to the change of the binding energy. The binding energy $E_{1s}^{B(l_e, l_h)}$ is shown in Fig. 3(b). We can see that, while the change in the binding energy also depends on the subbands, it is not large in the present region of F . Thus, the energy shift of excitons in Fig. 3(a) mainly comes from shifts of the electron and hole subband energies. Looking at detailed values of $\Delta E_i^{(l_i)}$ ($i = e$ or h) for the present hh exciton, we find the following points. The shift for the first subband $\Delta E_i^{(1)}$ is negative, while that of the second subband $\Delta E_i^{(2)}$ is positive and is small compared to $|\Delta E_i^{(1)}|$, as expected from the result in Sec. II. The magnitude of the shift for the hole $|\Delta E_h^{(l)}|$ is much larger than that for the electron $|\Delta E_e^{(l)}|$ because of the larger hole mass $m_{hz} = 0.353m_0$ compared to the electron mass $m_e = 0.067m_0$. The above points explain how the subband dependence of the energy shift arises in Fig. 3(a). In the experiments of the optical absorption^{3,9} we find the strong subband dependence of the energy shift. For example, from Fig. 1 and Table I in the work of Yamakaka *et al.*⁹ for GaAs-Ga_{0.66}Al_{0.34}As with $L = 105 \text{ \AA}$, we may obtain roughly the following values for $\Delta E_{1s}^{(l_e, l_h)}$ in meV: at $F = 6.5 \times 10^4 \text{ V/cm}$ ($1.1 \times 10^5 \text{ V/cm}$), $-7(-20)$ for $(l_e, l_h) = (1,1)$, $-5(-15)$ for $(2,1)$, $-3(-9)$ for $(1,2)$, and $0(-5)$ for $(2,2)$. This result of the strong subband dependence is in a good agreement with the presently calculated results qualitatively (or semiquantitatively if we consider $L = 120 \text{ \AA}$ to be the effective well width L_{eff}). For the further agreement (especially for higher subband excitons) the use of the finite potential barrier model (FPBM) seems to be necessary.

So far we have discussed the hh exciton. We have performed a similar calculation for the light-hole (lh) exciton, which has mass values $m_h = (\gamma_1 - \gamma_2)^{-1}m_0 = 0.191m_0$ and $m_{hz} = (\gamma_1 + 2\gamma_2)^{-1}m_0 = 0.080m_0$. Energy shifts for lh excitons are smaller compared to those for hh excitons, because of the smaller mass m_{hz} , and have a similar subband dependence as for hh excitons in a qualitative agreement with the experiment.⁹

Under electric fields, an electron and a hole, which constitute an exciton, receive the forces in the opposite directions. Then, the change in wave functions will appear directly in the oscillator strength. In Fig. 4(a) we have shown how the oscillator strength f_{1s} varies in the presence of the electric field. It is seen that for stronger electric fields the oscillator strength for the usually allowed exciton with $(l_e, l_h) = (1,1)$ or $(2,2)$ decreases, while f_{1s} for the usually forbidden exciton with $(1,2)$ or $(2,1)$ increases and becomes the same order of magnitude as that for the allowed exciton. As expected from Eq. (14), this behavior originates from changes in the wave functions of the electron and hole subband parts and the exciton relative motion part. The electron-hole overlap function $F(0)$, which reflects the change in subband wave functions directly, is shown in Fig. 4(b). We see that f_{1s} in Fig. 4(a) and $F(0)$ in Fig. 4(b) have a similar variation and thus the main change in f_{1s} comes from that in $F(0)$, although the change of the relative motion wave function is necessary to obtain the accurate values of f_{1s} .

In the experiments of the optical absorption³ and the photocurrent spectroscopy,⁹ exciton peaks due to the for-

bidden exciton appear for strong electric fields. Our calculated result of f_{1s} agrees with this appearance.¹⁹ Also the experimental optical absorption spectra³ show the decrease in the oscillator strength for the lowest (1,1) hh exciton for stronger electric fields in agreement with the present calculated result: by analyzing the spectra in the same way as done in the zero electric field case,²⁰ we find that the oscillator strength decreases by about 25% (30%) for the increase in the electric field from about 8 to 22 (39) kV/cm. We think that for the full quantitative comparison, the FPBM should be used.

From the picosecond spectroscopy of the luminescence spectra some experiments have deduced the lifetime of an exciton.^{6,7,10,11} The lifetime is inversely proportional to the oscillator strength. Then, the increase in the lifetime in Refs. 7 and 10 agrees qualitatively with the present calculation, although the decrease is found in Refs. 6 and 10. Probably, the difference arises from the structure of the quantum well. For the structure where the finite potential barrier and multi-QW effects (such as the tunneling through the barrier) are not so important, the increase should be observed.

IV. SUMMARY

We have considered electric field effects on subbands and excitons, in paying attention to their subband depen-

dence. Using the infinite potential barrier model, we have found that there is a strong subband dependence of the energy and the oscillator strength in the presence of the electric field. The calculated behavior agrees well with the experiment qualitatively (or semiquantitatively). In order to explain quantitatively excitonic properties with various electron and hole subbands in the experiments done so far, the finite potential barrier effect not only in a single quantum well⁵ but also in a multi-quantum well need to be studied fully. This is because the present model calculation is suitable to the case where both electron and hole are confined nearly perfectly even under electric fields. Also for the full calculation, effects of the hh and lh mixing²¹ should be taken into account, although in the present perpendicular electric field case the hole mass in z direction m_{hz} essentially determines electric field effects.

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