Excitons in type-II quantum-well systems: Binding of the spatially separated electron and hole

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Excitons in type-II quantum-well systems, i.e., in the configuration of the spatially separated electron and hole, are studied by the variational calculation of binding energies and spatial extensions with the use of the infinite-potential-barrier model. It is shown that (i) excitonic properties depend very much on the electron-hole mass ratio and the well widths and that (ii) the dimensional character of an exciton (such as two-dimensional 1s and the three-dimensional $2p_z$ character) appears in some limits of these physical parameters of the system.

I. INTRODUCTION

In recent years there has been great interest in studying excitonic properties of quantum-well (QW) or superlattice (SL) systems. Most studies have been performed in the QW structures where an electron and a hole are confined spatially in the same well because of the specific configuration of the conduction- and the valence-band edges [Fig. 1(a)]. This type of QW is called "type I" and has been studied extensively in the GaAs-$Al_xGa_{1-x}As$ system. For the smaller well width L_I, an exciton has quasi-two-dimensional character and has a larger binding energy and a larger oscillator strength.[1-6]

Another type of QW system, where an electron and a hole are confined in spatially separate wells [Fig. 1(b)], is called "type II." It is expected that the character of excitons in type-II QW systems is quite different from that in type-I QW systems. There have been a few studies of this problem. Lozovik and Nishanov[7] considered a system consisting of an electron and a hole which move in separate planes. Bastard *et al.*[1] studied excitons in the GaSb-InAs-GaSb double heterostructure [with $L_{II}=\infty$ in Fig. 1(b)] and obtained a reduction of the binding energy relative to the value of the two-dimensional exciton. Duggan and Ralph[8] calculated binding energies of X-point excitons, which belong to those of the type-II configuration, in the GaAs-AlAs SL structure and found a large binding energy comparable to the 1s heavy-hole Γ-point exciton in the type-I configuration in this system. So far, all the above-mentioned work treated only the individual specific cases.

In the present work we consider the problem from a general point of view. Using an infinite-potential-barrier model, we perform a variational calculation of excitons in type-II QW structures: the results of the binding energy and the spatial extension clarify the nature of exciton states for various physical parameters such as the masses of an electron and a hole and well widths.

II. CALCULATION AND DISCUSSION

Let us consider an exciton in type-II quantum-well systems which consist of two materials I and II with respective layer thicknesses L_I and L_{II} [Fig. 1(b)]. The z axis is taken to be perpendicular to the layers. One of the interfaces is chosen as the origin of the z coordinate. The exciton consists of an electron [mass m_e, position $\mathbf{r}_e=(x_e,y_e,z_e)$, momentum $\mathbf{p}_e=(p_{ex},p_{ey},p_{ez})$] and a hole [mass m_h, position $\mathbf{r}_h=(x_h,y_h,z_h)$, momentum $\mathbf{p}_h=(p_{hx},p_{hy},p_{hz})$]. The Hamiltonian of the system is written as

$$H=\frac{p_{ez}^2}{2m_e}+\frac{p_{hz}^2}{2m_h}+\frac{p_x^2+p_y^2}{2\mu}-\frac{e^2}{\epsilon r}+\Delta V^{\rm im}+V_e^{\rm conf}(z_e)+V_h^{\rm conf}(z_h)\ . \quad (1)$$

Here we omitted the center-of-mass motion in the x-y plane, whose free motion can be decoupled from the other motion. The position and momentum operators of the relative motion are denoted by $\mathbf{r}\equiv\mathbf{r}_e-\mathbf{r}_h=(x,y,z)$ and

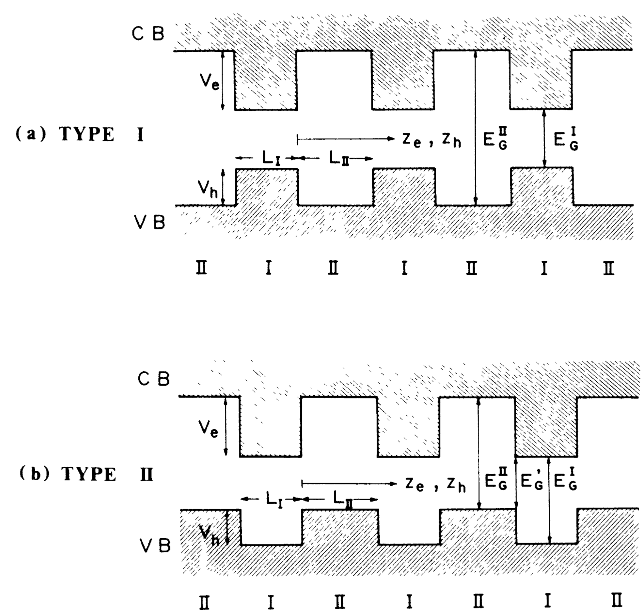

FIG. 1. Potential profile of (a) type-I and (b) type-II quantum-well structures.

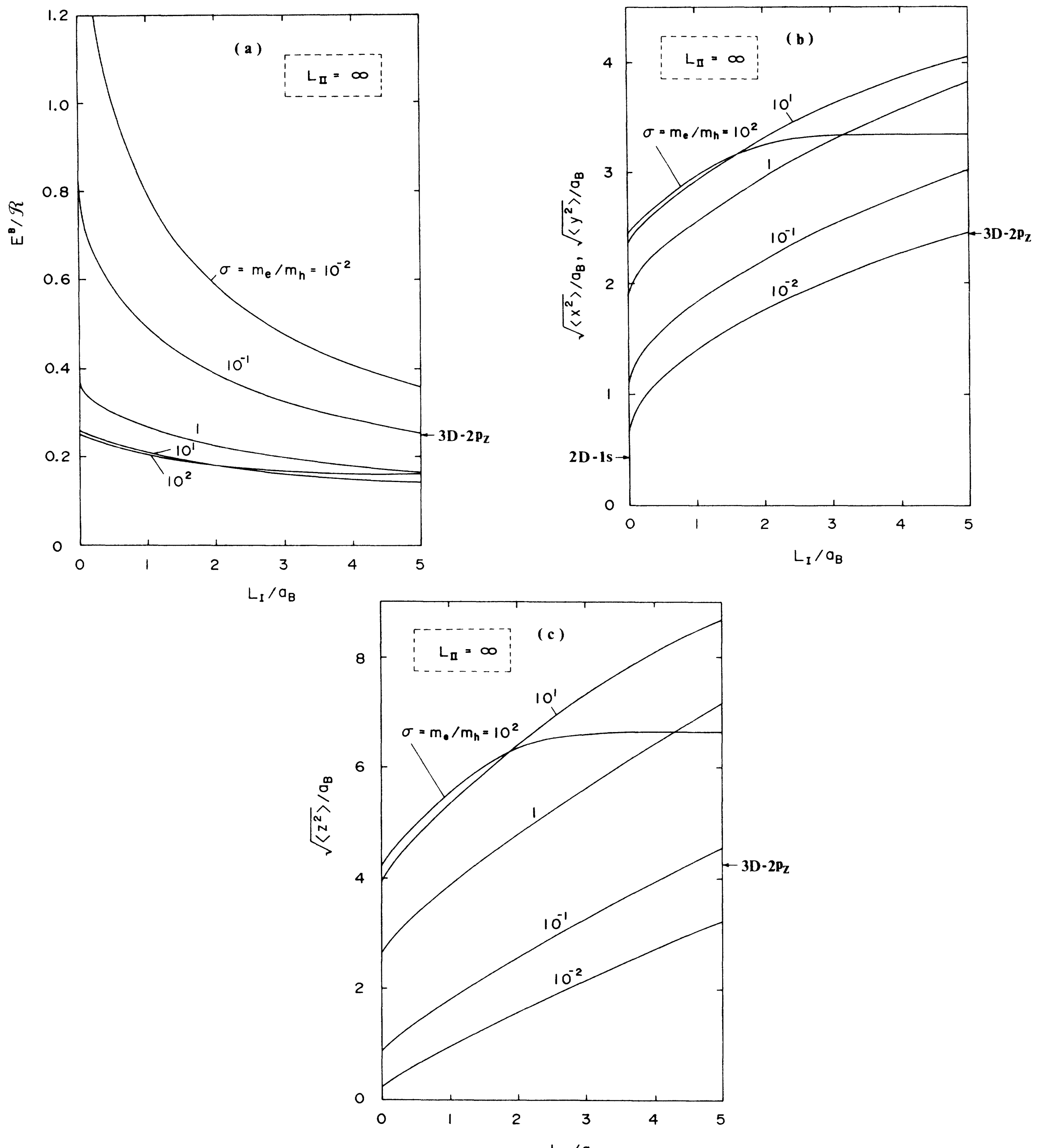

FIG. 2. (a) Exciton binding energy E^B and the spatial extensions (b) in the x and y directions $\sqrt{\langle x^2\rangle}=\sqrt{\langle y^2\rangle}$ and (c) in the z direction $\sqrt{\langle z^2\rangle}$ in the case of $L_{\mathrm{II}}=\infty$ as a function of the well width L_{I} for various values of the electron-hole mass ratio $\sigma=m_e/m_h$.

$\mathbf{p}=(p_x,p_y,p_z)$, respectively. The reduced mass is given by $\mu=m_e m_h/(m_e+m_h)$. The Coulomb interaction between an electron and a hole is described by the fourth term in the Hamiltonian (1) with $\epsilon=(\epsilon_{\mathrm{I}}+\epsilon_{\mathrm{II}})/2$, where ϵ_{I} and ϵ_{II} are the dielectric constants of the materials I and II, respectively. The difference of ϵ_{I} and ϵ_{II} produces an image-potential-type term (a dielectric mismatch potential) ΔV^{im}, which depends on the dielectric mismatch factor $q=(\epsilon_{\mathrm{I}}-\epsilon_{\mathrm{II}})/(\epsilon_{\mathrm{I}}+\epsilon_{\mathrm{II}})$.[9] In the present work we neglect the term ΔV^{im}. The confinement potentials $V_e^{\mathrm{conf}}(z_e)$ and $V_h^{\mathrm{conf}}(z_h)$ for an electron and a hole are given by

$$V_e^{\mathrm{conf}}(z_e)=\begin{cases}0 & \text{for } n_1L-L_{\mathrm{I}}<z_e<n_1L\\ V_e & \text{for } n_2L<z_e<n_2L+L_{\mathrm{II}}\end{cases}$$

and (2)

$$V_h^{\text{conf}}(z_h) = \begin{cases} V_h & \text{for } n_3L - L_{\text{I}} < z_h < n_3L \\ 0 & \text{for } n_4L < z_h < n_4L + L_{\text{II}}, \end{cases}$$

where $L = L_{\text{I}} + L_{\text{II}}$ and $n_i = 0, \pm 1, \pm 2, \ldots$. In the present work we use the infinite-potential-barrier model, i.e, $V_e, V_h \to \infty$ and then an electron and a hole are perfectly confined in the materials I and II, respectively. In the following we consider two different cases separately: (A) double-hetero-QW structures [with $L_{\text{II}} = \infty$ in Fig. 1(b)] and (B) superlattice structures [with finite L_{II} in Fig. 1(b)].

A. Double-hetero-QW structures ($L_{\text{II}} = \infty$ case)

In the present infinite-L_{II} case, if the Coulomb interaction between an electron and a hole is neglected, the electron motion in the z direction is quantized with the well width L_{I}, while a hole is in the band state. When the Coulomb attraction is taken into account, both particles approach the interface from the opposite directions. Keeping this situation in mind and considering the configuration of an electron in $-L_{\text{I}} < z_e < 0$ and a hole in $0 < z_h < \infty$, we use the following variational wave function for the lowest exciton:

$$\Phi_A = N_A \psi_e(z_e) f_e(z_e) f_h(z_h) \phi(x,y,z) \ . \quad (3)$$

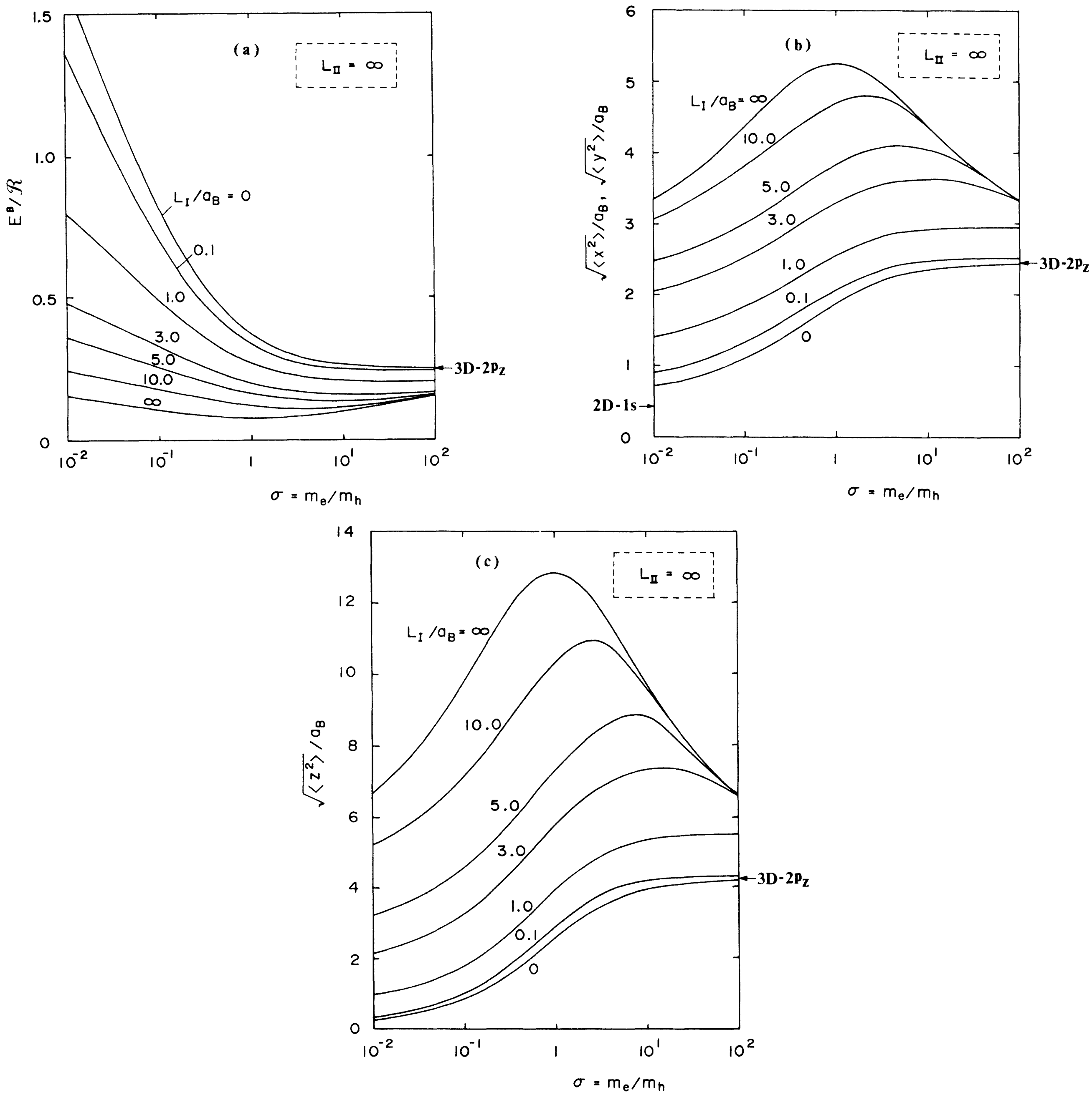

FIG. 3. (a) Exciton binding energy E^B and the spatial extensions (b) in the x, y directions $\sqrt{\langle x^2 \rangle} = \sqrt{\langle y^2 \rangle}$ and (c) in the z direction $\sqrt{\langle z^2 \rangle}$ in the case of $L_{\text{II}} = \infty$ as a function of the electron-hole mass ratio $\sigma = m_e/m_h$ for various values of the well width L_{I}.

Here, N_A is the normalization constant,

$$\psi_e(z_e)=\sqrt{1/L_{\rm I}}\sin(\pi z_e/L_{\rm I})$$

is the subband wave function of an electron, and

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

describes the relative motion. The functions $f_e(z_e)=\exp(\beta_e z_e)$ and $f_h(z_h)=z_h\exp(-\beta_h z_h)$ represent a modulation of z-directional motions of an electron and a hole due to the exciton effect. The four variational parameters α, β, β_e, and β_h are determined from the minimization of the energy $E=\langle\Phi_A|H|\Phi_A\rangle$. The obtained exciton energy $E_{\rm ex}$ determines the binding energy of an exciton from $E^B=E_\infty-E_{\rm ex}$, where $E_\infty=\pi^2\hbar^2/2m_eL_{\rm I}^2$ is the electron subband energy.

If we normalize the length by the Bohr radius a_B ($\equiv\epsilon\hbar^2/\mu e^2$) and the energy by the Rydberg energy $\mathcal{R}$ ($\equiv\mu e^4/2\epsilon^2\hbar^4$), the present system can be characterized by the electron-hole mass ratio $\sigma\equiv m_e/m_h$ and the well width $L_{\rm I}$. For various values of these physical parameters, the exciton binding energy E^B is calculated. We also calculate spatial extensions of an exciton in the x,y directions $\sqrt{\langle x^2\rangle}=\sqrt{\langle y^2\rangle}$ and in the z direction $\sqrt{\langle z^2\rangle}$. The calculated results are shown in Figs. 2 and 3.

Let us discuss exciton states of the present configuration with $L_{\rm II}=\infty$. As we see below, a nature of excitons depends strongly on the electron-hole mass ratio σ and the well width $L_{\rm I}$. The following two-dimensional (2D) or three-dimensional (3D) character is expected:

$$\begin{aligned}L_{\rm I}\to 0,\quad & \text{2D 1}s\text{ type } (E^B=4\mathcal{R})\ \text{ for } \sigma\ll 1\\ & \text{3D }2p_z\text{ type } (E^B=\tfrac{1}{4}\mathcal{R})\ \text{ for } \sigma\gg 1\ ,\\ L_{\rm I}\to\infty,\quad & \text{3D }2p_z\text{ type } (E^B=\tfrac{1}{4}\mathcal{R})\\ & \text{for } \sigma\gg 1 \text{ and } \sigma\ll 1\ .\end{aligned}\tag{4}$$

The reasons why we expect the above behavior of excitons are as follows. When the well width $L_{\rm I}$ approaches zero, the z coordinate of an electron is fixed. Then, for very large hole mass ($\sigma\ll 1$), an exciton becomes 2D 1s type, because a hole approaches very close to the interface. On the other hand, for very small hole mass ($\sigma\gg 1$) a hole can be away from the interface and then an exciton becomes 3D $2p_z$ type: the situation is the same as that of a bound electron in a Coulombic impurity at the surface, whose ground state is the 3D $2p_z$ type.[10] When the well width $L_{\rm I}$ is very large and $\sigma\gg 1$, an electron approaches very close to the interface, while a hole does not. Then an exciton becomes 3D $2p_z$ type as in the case of $\sigma\gg 1$ for the $L_{\rm I}\to 0$ limit. A similar 3D $2p_z$-type exciton also occurs for large $L_{\rm I}$ and $\sigma\ll 1$, where a hole is very close to the interface. This behavior is realized only when σ is very small or very large, as seen in Figs. 2 and 3.

The figures also show how the character of excitons in type-II double-hetero-QW structures depends on the physical parameters $L_{\rm I}$ and σ, generally. The following points can be seen. First, when the well width $L_{\rm I}$ becomes small, the 2D 1s-type character such as a large binding energy appears very strongly for small σ and this character becomes weaker with the increase of σ. For large σ excitons become 3D $2p_z$ type. Thus, excitons change their character remarkably according to the change of σ when $L_{\rm I}/a_B$ is smaller than 1. Second, when $L_{\rm I}/a_B$ is larger than 3, the dependence of E^B on σ is small and the excitons keep their 3D $2p_z$-type character to some extent for any σ

Above we have considered the nonsymmetrical configuration of an exciton: an electron in the region of $-L_{\rm I}<z_e<0$ and a hole in the region of $0<z_h$. We can also consider the symmetrical configuration of an electron in the region of $-L_{\rm I}<z_e<0$ and a hole in the region of $z_h<-L_{\rm I}$ and $0<z_h$, as considered in Ref. 1. For the symmetrical configuration, we choose the form of $f_e(z_e)$ and $f_h(z_h)$ in the variational wave function (3) as

$$f_e(z_e)=\exp\left[b_e\left[z_e+\frac{L_{\rm I}}{2}\right]\right]+\exp\left[-b_e\left[z_e+\frac{L_{\rm I}}{2}\right]\right]\quad\text{for } -L_{\rm I}<z_e<0\tag{5}$$

and

$$f_h(z_h)=\left[\left|z_h+\frac{L_{\rm I}}{2}\right|-\frac{L_{\rm I}}{2}\right]\exp\left[-b_h\left|z_h+\frac{L_{\rm I}}{2}\right|\right]\quad\text{for } z_h<-L_{\rm I}\text{ and } z_h>0\ .\tag{6}$$

The calculation for the symmetrical configuration is performed and the results obtained are quite similar to those for the nonsymmetrical one: the differences of the binding energies are less than 0.1% and in some parameter regions the symmetrical configuration yields lower energies, while in other regions it does not. The spatial extensions for both configurations are also quite similar, though the values of $\sqrt{\langle z^2\rangle}$ in the symmetrical configuration are slightly larger than those in the nonsymmetrical one for large $L_{\rm I}$ and large σ. From these results we conclude that the choice of the configuration does not change the features of the present results in Figs. 2 and 3.

B. Superlattice structure (finite-$L_{\rm II}$ case)

Now we consider the finite-$L_{\rm II}$ case, where both an electron and a hole are in subband states. For the variational wave function of the lowest exciton, which consists of an electron ($-L_{\rm I}<z_e<0$) and a hole ($0<z_h<L_{\rm II}$), we use

$$\Phi_B = N_B \psi_e(z_e)\psi_h(z_h) f_e(z_e) f_h(z_h)\phi(x,y,z) \ . \tag{7}$$

Here, N_B is the normalization constant;

$$\psi_e(z_e) = (1/L_{\mathrm{I}})^{1/2}\sin(\pi z_e/L_{\mathrm{I}})$$

and

$$\psi_h(z_h) = \sqrt{1/L_{\mathrm{II}}}\sin(\pi z_h/L_{\mathrm{II}})$$

are the subband wave functions of an electron and a hole, respectively;

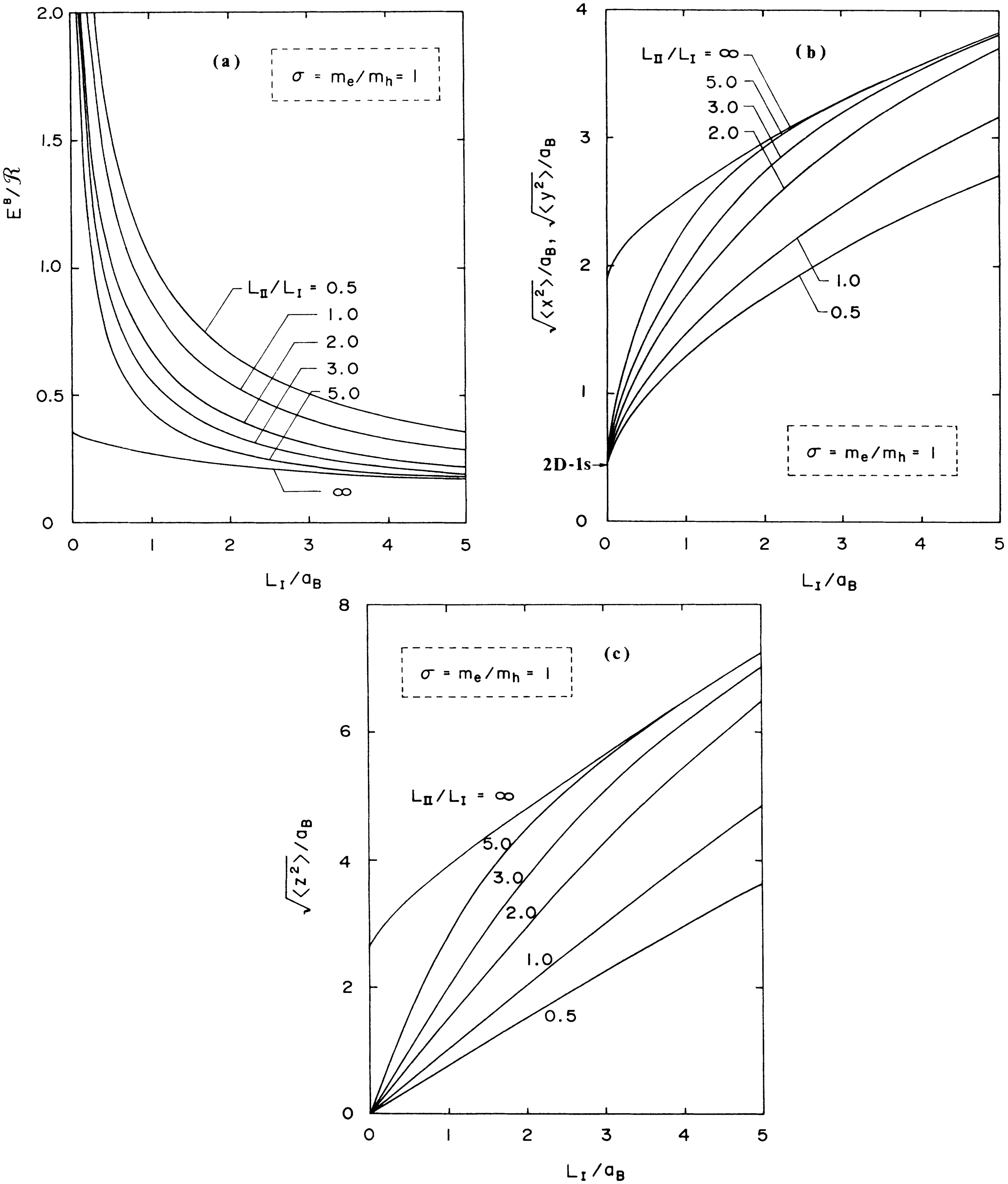

FIG. 4. (a) Exciton binding energy E^B and the spatial extensions (b) in the x, y, directions $\sqrt{\langle x^2\rangle}=\sqrt{\langle y^2\rangle}$ and (c) in the z direction $\sqrt{\langle z^2\rangle}$ in the finite L_{II} case as a function of the well width L_{I} for various values of the well-width ratio $L_{\mathrm{II}}/L_{\mathrm{I}}$ and the fixed value of the electron-hole mass ratio $\sigma=1$.

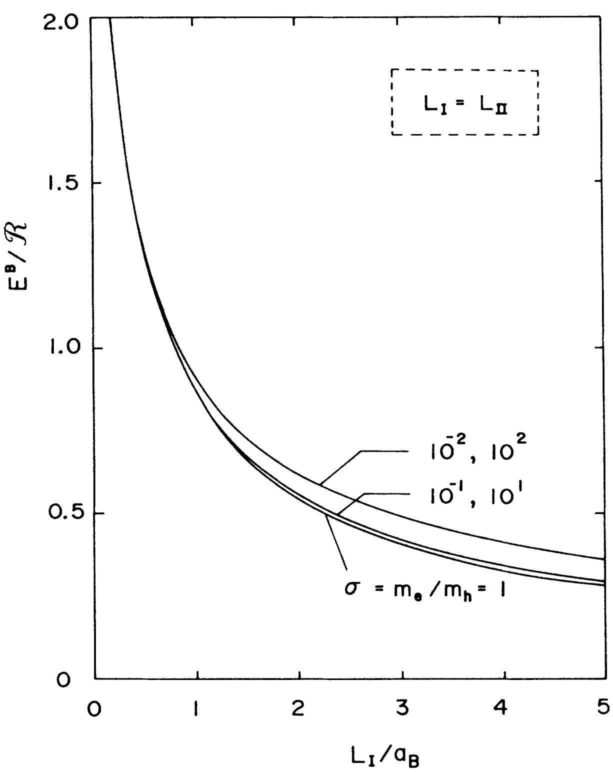

FIG. 5. Exciton binding energy E^B in the finite L_{II} case as a function of the well width L_I for the various values of the electron-hole mass ratio $\sigma = m_e/m_h$ and the fixed values of $L_I = L_{II}$.

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

describes the relative motion. We choose

$$f_e(z_e) = \exp(\beta_e z_e)$$

and

$$f_h(z_h) = \exp(-\beta_h z_h)$$

as modulation functions of the z-directional motions of an electron and a hole due to the exciton effect. After the minimization of the energy $E = \langle \Phi_B | H | \Phi_B \rangle$ with respect to four variational parameters α, β, β_e, and β_h, we obtain the exciton energy E_{ex} and then the exciton binding energy from $E^B = E_\infty - E_{ex}$, where

$$E_\infty = \pi^2\hbar^2/2m_e L_I^2 + \pi^2\hbar^2/2m_h L_{II}^2$$

is the sum of the subband energies of an electron and a hole. The spatial extensions of excitons $\sqrt{\langle x^2 \rangle} = \sqrt{\langle y^2 \rangle}$ and $\sqrt{\langle z^2 \rangle}$ are also calculated. If the Bohr radius a_B for the length and the Rydberg energy $\mathcal{R}$ for the energy are used for units as in the case (A), the present system (B) can be characterized by the three physical parameters: the electron-hole mass ratio σ and the well widths L_I and L_{II}. The calculated results for various values of σ, L_I, and L_{II} are shown in Figs. 4–6.

Now we discuss the results. In some limits, we expect the following dimensional character for excitons from the reasons similar to the case (A):

$$\begin{aligned}
&L_I \text{ and } L_{II} \to 0,\ \text{2D 1}s \text{ type } (E^B = 4\mathcal{R}) \\
&\qquad\qquad\qquad \text{for any values of } \sigma; \\
&L_I \to 0 \text{ and } L_{II} \to \infty,\ \text{2D 1}s \text{ type } (E^B = 4\mathcal{R}) \text{ for } \sigma \ll 1 \\
&\text{3D } 2p_z \text{ type } (E^B = \tfrac{1}{4}\mathcal{R}) \text{ for } \sigma \gg 1; \\
&L_I \to \infty \text{ and } L_{II} \to 0, \text{3D } 2p_z \text{ type } (E^B = \tfrac{1}{4}\mathcal{R}) \\
&\qquad\qquad\qquad \text{for } \sigma \ll 1 \\
&\text{2D 1}s \text{ type } (E^B = 4\mathcal{R}) \text{ for } \sigma \gg 1; \\
&L_I \text{ and } L_{II} \to \infty,\ \text{3D } 2p_z \text{ type } (E^B = \tfrac{1}{4}\mathcal{R}) \\
&\qquad\qquad\qquad \text{for } \sigma \gg 1 \text{ and } \sigma \ll 1 .
\end{aligned} \tag{8}$$

Figures 4–6 show the general nature of excitons for various values of the physical parameters of the system and the above character of excitons in some limits is seen. In the figures we notice the following points. The nature of excitons depends strongly on the well-width ratio L_{II}/L_I. When L_{II}/L_I is smaller, the 2D 1s-type character such as a large binding energy and a small exciton radius (i.e., small $\sqrt{\langle x^2 \rangle}$ and $\sqrt{\langle y^2 \rangle}$) appears very strongly for the small well width L_I and for any electron-hole mass ratio σ. When L_{II}/L_I is larger, we have more or less the 3D $2p_z$-type character for large L_I. When both well widths L_I and L_{II} are smaller, the exciton state depends less on σ.

III. SUMMARY

In the present work, using an infinite-potential-barrier model, we have performed a variational calculation of excitons in type-II QW structures and have clarified the nature of excitons from a general point of view. It has been shown that (i) excitons in type-II QW structures are very different from those in type-I QW structures and depend very much on the electron-hole mass ratio σ and the well widths L_I and L_{II} and that (ii) a dimensional character of excitons appears for some limiting values of these physical parameters.

Finally we discuss the validity of the present result which has been obtained with the use of the infinite-potential-barrier model. When the potential barriers are finite, an exciton wave function is no longer confined in the well. The amount of the spread of exciton wave functions into the barriers is mainly determined by that of the subband wave functions of an electron and a hole. It is well known that the spread of the subband wave functions increases for smaller $V_e L_I^2$ $(V_h L_{II}^2)$: for example, for $2m_e V_e L_I^2/\pi^2\hbar^2$ $(2m_h V_h L_{II}^2/\pi^2\hbar^2) = 1.5$ (0.5) the probabilities for finding an electron (a hole) in the well part are 0.89 (0.72). Therefore, the result of the present work is valid when $2m_e V_e L_I^2/\pi^2\hbar^2$ and $2m_h V_h L_{II}^2/\pi^2\hbar^2$

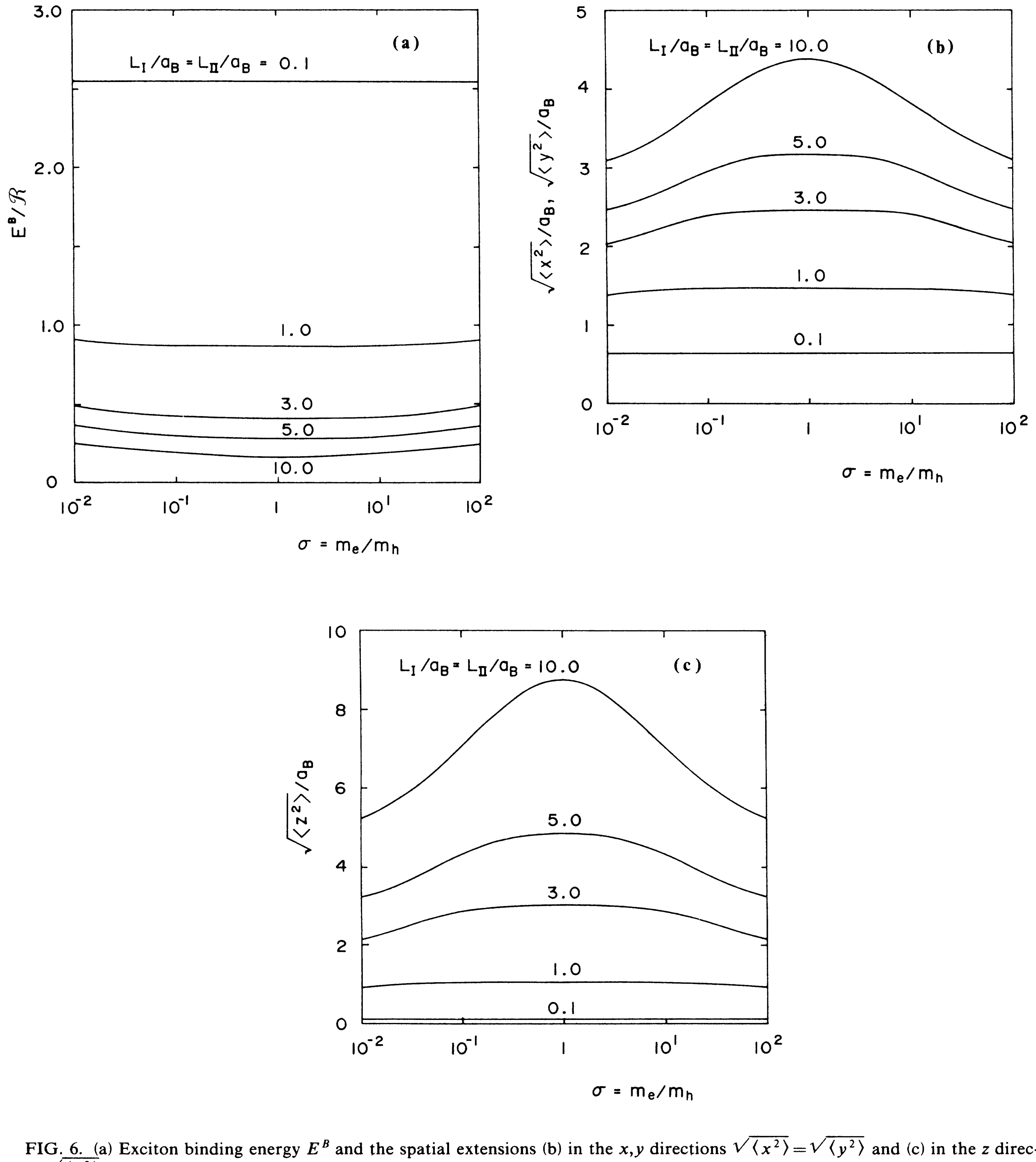

FIG. 6. (a) Exciton binding energy E^B and the spatial extensions (b) in the x,y directions $\sqrt{\langle x^2\rangle}=\sqrt{\langle y^2\rangle}$ and (c) in the z direction $\sqrt{\langle z^2\rangle}$ in the finite L_{II} case as a function of the electron-hole mass ratio $\sigma=m_e/m_h$ for various values of the well width $L_{\mathrm{I}}=L_{\mathrm{II}}$.

are larger than ~ 1.5. For small $V_e L_{\mathrm{I}}^2$ and $V_h L_{\mathrm{II}}^2$, the spread of the exciton wave function changes the character of excitons. For instance, if the potential barrier heights are fixed, the spilling of the exciton wave function into barrier parts becomes important for smaller well widths beyond a certain value. In this situation, the 3D 1s character of the exciton starts to increase and we lose character of 2D 1s or 3D 2p_z type, for some limits of the present calculation. A similar change in character (2D 1s type $\leftrightarrow$3D 1s type) also occurs in type-I QW systems.[2] In general, the finite-potential-barrier effect is important and should be studied as the next step for the present exciton problem. Another effect of the finite potential barrier is a nonzero oscillator strength; this is interesting in connection with optical properties of type-II systems. For comparison with experiments on real physical systems, it will also be necessary to consider the image-potential-type term ΔV^{im} as well as the band complexity, which includes the anisotropy of the hole mass, nonparabolicity, and the mixing of the light- and heavy-hole subbands.

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