Donors and excitons in triangular GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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We present in this paper a variational calculation for the ground state of the donor and light- and heavy-hole excitons in triangular quantum wells. The binding energy and the lateral and vertical extensions of the wave function are calculated for several well-height values, all as functions of the well width. Compared with a square-well structure or a δ-doped well, the triangular quantum well presents a greater restriction to the donor and exciton. As a result, the lateral and vertical extensions of the ground state are smaller, while the binding energy and the probability inside the well are larger. We conclude in this paper that a triangular quantum-well structure may be significant for theoretical research and practical application.

I. INTRODUCTION

Gossard *et al.*[1] have grown triangular quantum barriers using molecular-beam epitaxy. Obviously, a triangular quantum well can also be grown using the same technique. Suppose there is such a structure to be grown, whose potential is shown in Fig. 1. Region I ($|z|>b$) is $Ga_{1-x}Al_xAs$, and region II ($-b<z<b$) is $Ga_{1-y}Al_yAs$. In region II the Al concentration y varies with $|z|$, so that the band-edge profile is triangular, with $y=0$ at the quantum-well center. Note that, for both the electron and hole, the potential is a triangular barrier in this model. First, we use the variational method to calculate the ground-state binding energies for the donor and heavy- and light-hole excitons. We then calculate the lateral and vertical extension of the exciton. The results are expressed as a function of quantum-well width for several values of potential-well heights (or the Al concentration x in region I). Finally, we compare the results with those for a δ-doped well and a square well. In the δ-doped structure, for the electrons the effective potential is a triangular well, while for the holes it is a triangular barrier. Our results for the donor for large x and small width are similar to those of Crowne, Reinecke, and Shanabrook[2] (for an infinite triangular δ-doped potential well). Our results differ, however, from those of a square well.

II. THEORY

In a cylindrical coordinate system, the Hamiltonian of a donor in the center of a triangular quantum well (within the framework of the effective-mass approximation) is

$$H=-\frac{\hbar^2}{2m_e}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}\right]-\frac{e^2}{\epsilon(\rho^2+z^2)^{1/2}}+V_{\rm tr} \quad (1)$$

Here the origin of coordinates 0 coincides with the well center, as shown in Fig. 1. m_e is the effective mass of the conduction electron and ϵ the static dielectric constant. For the conduction electron, the potential well is

$$V_{\rm tr}=\begin{cases}V_e|z|/b, & -b<z<b,\\ V_e, & |z|>b,\end{cases} \quad (2)$$

where V_e and V_h, the potential-well height for the hole, are assumed to be about 60% and 40% of the total

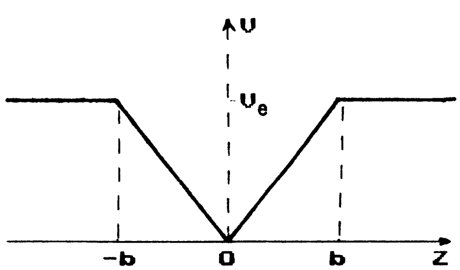

FIG. 1. Triangular quantum well potential profile along the z axis.

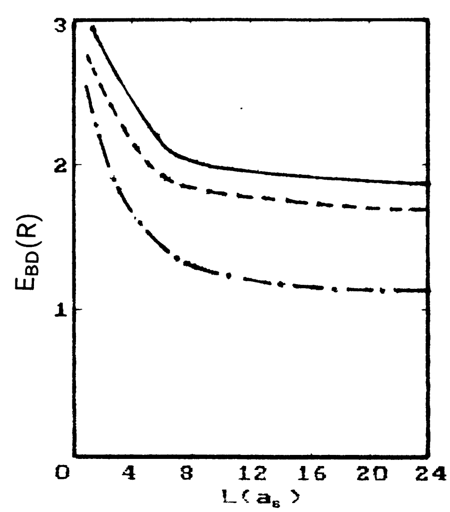

FIG. 2. Variation of E_{BD}, the binding energy of the donor ground state, as a function of the well width L at Al concentration $x=0.96$ (solid line), 0.37 (dashed line), and 0.041 (dot-dashed line).

energy-band-gap difference between $|z|=b$ and $z=0$.

In this paper, we have chosen to use the effective Bohr radius a_B as the length unit and the effective Rydberg R as the energy unit. According to a variational approach, we use the following trial wave function:

$$\psi_D=f_e(z)g(\rho,z,\phi)\ , \tag{3}$$

where the function $f_e(z)$ is the exact (unnormalized) ground-state solution to the finite triangular well problem. It can be written as

$$f_e(z)=\begin{cases} c_1\mathrm{Ai}[(V_e/b)^{1/3}(z-bE_e/V_e)]+c_2\mathrm{Bi}[(V_e/b)^{1/3}(z-bE_e/V_e)], & 0<z<b,\\ c_3\mathrm{Ai}[(V_e/b)^{1/3}(-z-bE/V)]+c_4\mathrm{Bi}[(V_e/b)^{1/3}(-z-bE_e/V_e)], & -b<z<0,\\ c_5\exp[-(V_e-E_e)^{1/2}(|z|-b)], & |z|>b. \end{cases} \tag{4}$$

Here, $\mathrm{Ai}(x)$ and $\mathrm{Bi}(x)$ are Airy functions. E_e is the energy of the lowest conduction-electron subband. c_1, c_2, c_3, c_4, c_5, and E_e are obtained from the continuity conditions of $f_e(z)$ and its first derivative at the interface ($z=0, |z|=b$). The function $g(\rho,z,\phi)$ for the ground state of the donor is

$$g(\rho,z,\phi)=N\exp[-(\rho^2/\alpha^2+z^2/\beta^2)^{1/2}]\ . \tag{5}$$

Here N is the normalization constant, and α and β are variational parameters. We first evaluate the expectation value of H_D at the donor ground state, i.e. (assuming the wave function is normalized),

$$E_D=\int\int\int \psi_D^* H_D \psi_D \rho\, d\rho\, dz\, d\phi\ , \tag{6}$$

and minimize this expression as a function of α and β. The donor binding energy E_{BD} of the ground state is now obtained by subtracting E_D from the lowest electron-subband energy E_e, i.e., $E_{BD}=E_e-E_D$.

We then calculate the binding energies of the ground states of heavy- and light-hole excitons in a triangular quantum well. The exciton Hamiltonian can be expressed as

$$H=-\frac{\hbar^2}{2\mu_\pm}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\rho^2}\right]-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2}-\frac{\hbar^2}{2m_\pm}\frac{\partial^2}{\partial z_h^2}-\frac{e^2}{\epsilon|\mathbf{r}_e-\mathbf{r}_h|}+V_{\rm tr}^e+V_{\rm tr}^h\ . \tag{7}$$

Here $m_\pm$ are the heavy- and light-hole mass along the z direction, and $\mu_\pm$ is the reduced mass corresponding to the heavy- and light-hole bands in the plane perpendicular to the z axis. The positions of the electron and hole are indicated by $\mathbf{r}_e$ and $\mathbf{r}_h$ respectively, with ρ, z, and ϕ the relative electron-hole coordinates. $V_{\rm tr}^e$ is similar to $V_{\rm tr}$ of Eq. (2), but takes z_e as its variable. $V_{\rm tr}^h$ can be expressed as

$$V_{\rm tr}^h=\begin{cases} V_h|z_h|/b, & -b<z_h<b,\\ V_h, & |z_h|>b. \end{cases} \tag{8}$$

Now we shall take a variational approach and use the following form for the trial wave function of the exciton ground state:

$$\psi=f_e(z_e)f_h(z_h)g(\rho,z,\phi)\ . \tag{9}$$

The functions $f_e(z_e)$ for the electron and $f_h(z_h)$ for the

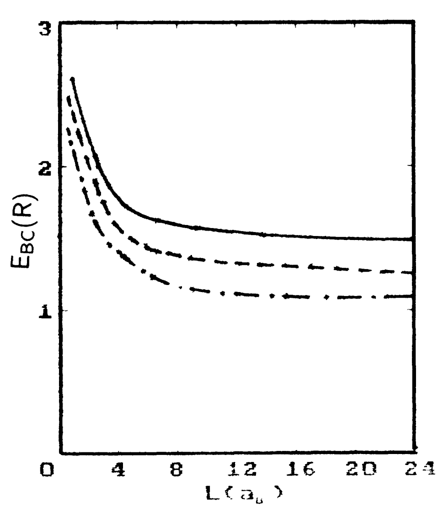

FIG. 3. Variation of E_{BC}, the binding energy of the ground state of a light-hole exciton, as a function of L at $x=0.96$ (solid line), $x=0.37$ (dashed line), and $x=0.041$ (dot-dashed line).

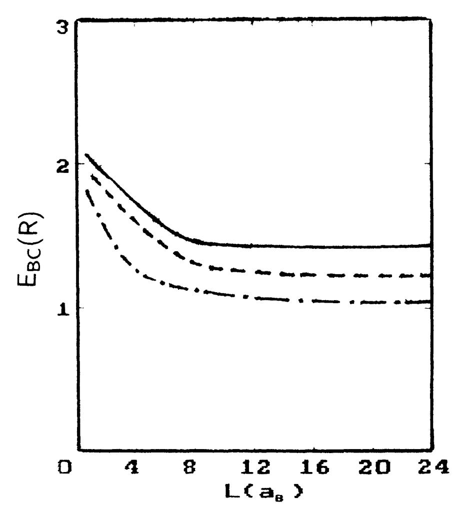

FIG. 4. Variation of E_{BC}, the binding energy of the ground state of a heavy-hole exciton, as a function of L at $x=0.96$ (solid line), $x=0.37$ (dashed line), and $x=0.041$ (dot-dashed line).

hole are the exact (unnormalized) ground-state solutions to the finite triangular well problem. $f_e(z_e)$ is similar to $f_e(z)$ of Eq. (4), but takes z_e as its variable. $f_h(z_h)$ can be written as

$$f_h(z_h)=\begin{cases} c_1'\mathrm{Ai}[(V_h'/b)^{1/3}(z_h-bE_h/V_h)]+c_2'\mathrm{Bi}[(V_h'/b)^{1/3}(z_h-bE_h/V_h)], & 0<z_h<b \\ c_3'\mathrm{Ai}[(V_h'/b)^{1/3}(-z_h-bE_h/V_h)]+c_4'\mathrm{Bi}[(V_h'/b)^{1/3}(-z_h-bE_h/V_h)], & -b<z_h<0, \\ c_5'\exp[-(V_h-E_h)^{1/2}(|z_h|-b)], & |z_h|>b. \end{cases} \quad (10)$$

Here E_h is the energy of the lowest hole subband, and c_1', c_2', c_3', c_4', c_5', and E_h are obtained by the continuity conditions of $f_h(z_h)$ and its first derivative at the interface ($z_h=0, |z_h|=b$). In order to employ the electron effective Bohr radius as length unit and the electron effective Rydberg as energy unit, we take $V_h'=V_h m_\pm/m_e$. The function $g(\rho,z,\phi)$ is the same as in Eq. (5). The expectation value of H at the exciton ground state can then be obtained:

$$E_C=\int\int\int\int \psi^* H\psi\rho\, d\rho\, dz_e dz_h d\phi\ , \quad (11)$$

and we minimize this expression as a function of α and β. Finally, the exciton binding energy E_{BC} of the ground state is obtained by subtracting E_C from E_e and E_h, i.e., $E_{BC}=E_e+E_h-E_C$.

III. RESULTS AND DISCUSSION

In Fig. 2 we demonstrate the variation of E_{BD}, the binding energy of the donor ground state, as a function of the triangular well width L ($=2b$) at $x=0.96$, 0.37, and 0.041. Crowne, Reinecke, and Shanabrook[2] have obtained results for a donor in an infinite δ-doped triangular well. Although our results are different from theirs in general for large values of x and small values of well width L both are similar. Further, our results are much different from the ones for a square quantum well (see, e.g., Chaudhuri and Bajaj[3]). In general, the binding energy of the donor ground state in a triangular well is much more than in a square well.

In Figs. 3 and 4 we give the variation of E_{BC}, the binding energy of the ground state of the light- and heavy-hole excitons, as a function of L at $x=0.96$, 0.37, and 0.041, respectively. These results are different from those for a square quantum well (see, e.g., Greene, Bajaj, and Phelps[4]) and for a δ-doped quantum well (see, e.g., Proetto[5]). Our results, in general, give larger energies than those in a square well, and much larger energies than those in a δ-doped well.

The electrons and holes in square quantum-well structures are acted upon by the potential barrier only outside the well, and so are free inside the well. In a triangular quantum-well structure, however, the electrons and holes are acted upon by the potential barriers both outside and inside the well. To demonstrate the effects of this confinement in the triangular well, we calculate the probability of finding an exciton inside the well, defined as

$$P=\int_0^\infty \int_{-b}^{b} \int_{-b}^{b} \int_0^{2\pi} \psi^*\psi\rho\, d\rho\, dz_e dz_h d\phi\ . \quad (12)$$

In Fig. 5 we plot the variation of P for the heavy-hole exciton as a function of L at $x=0.96$, 0.37, and 0.041. Compared with the results of Greene, Bajaj, and Phelps[4] our results are larger. This means that an exciton in a triangular quantum-well structure is confined much more than one in a square quantum-well structure. As for Fig. 6, it presents the lateral extension of the light-hole exciton $\langle\rho^2\rangle^{1/2}$ and the z-direction extension $\langle(z_e-z_h)^2\rangle^{1/2}$, both as functions of L at $x=0.37$. We find that these two extensions are much less than those in a δ-doped quantum-well structure. In a δ-doped quantum-well structure, the effective potential for the electrons is a potential well, while for the holes it is a potential barrier; as a result the extension of the exciton is larger. But in our structure the effective potential is a potential well for both the electrons and holes, so the extension is smaller. The reduced extension serves to increase the ground-state binding energies of the donor and exciton.

In summary, the ground-state binding energies of the donor and excitons in triangular quantum-well structures

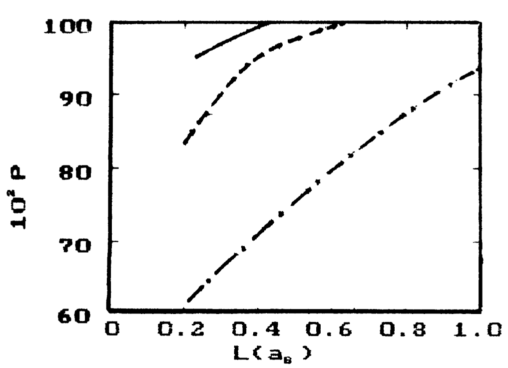

FIG. 5. Probability P of finding the heavy-hole exciton inside the well, as a function of L at $x=0.96$ (solid line), $x=0.37$ (dashed line), and $x=0.041$ (dot-dashed line).

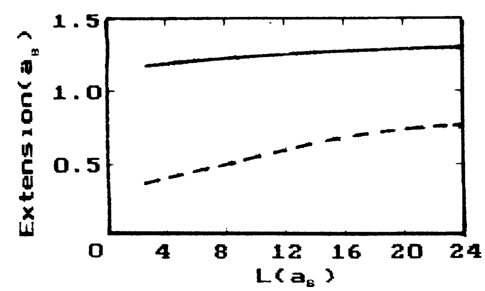

FIG. 6. Extension of light-hole exciton in plane $\langle\rho^2\rangle^{1/2}$ (solid line) and in the z direction $\langle(z_e-z_h)^2\rangle^{1/2}$ (dashed line) as a function of L at $x=0.37$.

are greater than in other structures (e.g., square quantum wells, δ-doping triangular quantum wells). In our structure the lateral extension and the z-direction extension of the exciton are smaller than in other structures. The probability of finding the exciton inside the well is greater than in other structures. Hence triangular quantum-well structures may be significant for theoretical research and practical applications.

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