Binding energies of Wannier excitons in GaAs-$Ga_{1-x}Al_xAs$ quantum-well structures in a magnetic field

Ronald L. Greene
Department of Physics, University of New Orleans, New Orleans, Louisiana 70148

K. K. Bajaj
U.S. Air Force Wright Aeronautical Laboratories, Avionics Laboratory (AFWAL/AADR), Wright-Patterson Air Force Base, Dayton, Ohio 45433

(Received 29 October 1984)

Binding energies of the ground state of both the heavy-hole and light-hole excitons in a GaAs quantum well sandwiched between two semi-infinite layers of $Ga_{1-x}Al_xAs$, are calculated as a function of the size of the well in the presence of an arbitrary magnetic field. A variational approach is followed where the trial wave functions are expressed in terms of Gaussian basis sets. The applied magnetic field is assumed to be parallel to the axis of growth and the binding energies are calculated for a finite value of the height of the potential barrier. As expected, for a given value of the magnetic field, the binding energies are found to be larger than their values in a zero magnetic field. The contribution to the binding energy due to the magnetic field, at a given field, increases slowly as the well size is reduced. A comparison with the available experimental data is made.

INTRODUCTION

The study of Wannier excitons in a quantum-well structure consisting of a single layer of GaAs sandwiched between two semi-infinite (generally larger than 200 Å in practice) layers of $Ga_{1-x}Al_xAs$ has attracted a great deal of interest in recent years.[1-9] Owing to the reduction in symmetry along the axis of growth and the presence of conduction- and valence-band discontinuities at the interfaces, the degeneracy of the valence band of GaAs is removed. This leads to the formation of two exciton systems associated with the two valence bands, namely, the heavy-hole exciton and the light-hole exciton. Miller *et al.*[3] calculated the binding energies of the ground state ($1S$) and of an excited state ($2S$), and later Bastard *et al.*[4] also calculated the binding energy of the ground state, of these excitons as a function of the well size (L) using infinite potential barriers at the interfaces. Both these groups followed a variational approach using different trial wave functions and obtained essentially the same results. Greene and Bajaj[5,7] were the first to calculate the binding energies of the ground state and of several excited states of both even and odd parity, of a heavy-hole and a light-hole exciton as a function of well size for finite values of the potential barrier. They found that both the magnitude and the qualitative behavior of the energy levels calculated using finite barrier heights were quite different from those obtained using infinite barriers, especially for thin ($L < 100$ Å) wells. Recently Shinozuka and Matsuura[6] have also calculated these energy levels using an infinite potential barrier. Using a variational-perturbation method, Jiang[8] has calculated the binding energies of the ground state of these excitons for finite barrier heights. In addition, several groups[1-3,9,10] have reported measurements of the binding energies of these excitons.

In this paper we report a calculation of the binding energies of the ground state (from hereon referred to as binding energies) of both the heavy-hole exciton and the light-hold exciton in a GaAs-$Ga_{1-x}Al_xAs$ quantum well as a function of the size of the GaAs well in the presence of an arbitrary magnetic field. We follow a variational approach in which the trial wave functions are expressed in terms of Gaussian basis sets. We assume that the applied magnetic field is parallel to the axis of growth and calculate the binding energies for finite values of the height of the potential barrier. As expected, we find that for a given value of the magnetic field, the binding energies are larger than their values in a zero magnetic field. In addition, the contribution to the binding energy due to the magnetic field, at a given field, increases slowly as the well size is reduced. We compare our results with the available experimental data.

THEORY

The Hamiltonian of an excitonic system in a GaAs layer sandwiched between two semi-infinite layers of $Ga_{1-x}Al_xAs$ grown along the [001] direction can be expressed, within the framework of an effective-mass approximation,[11] as

$$H = H_e\left[-i\hbar\nabla + \frac{e}{c}\mathbf{A}\right] - H_h\left[i\hbar\nabla + \frac{e}{c}\mathbf{A}\right] - \frac{e^2}{\epsilon_0 r} + V_{ew}(z_e) + V_{hw}(z_h)\ . \quad (1)$$

Here $\mathbf{A}$ is the vector potential associated with the magnetic field $\mathbf{B}$, ϵ_0 is the static dielectric constant of GaAs, H_e is the conduction-band Hamiltonian and H_h is the valence-band Hamiltonian. The explicit expression for H_e is

$$H_e=\frac{1}{2m_e}\left[-i\hbar\nabla+\frac{e}{c}\mathbf{A}\right]^2 \tag{2}$$

and H_h is described by the well-known Kohn-Luttinger Hamiltonian.[12] The relative coordinate $\mathbf{r}=\mathbf{r}_e-\mathbf{r}_h$, where $\mathbf{r}_e$ and $\mathbf{r}_h$ are the positions of the electron and hole, respectively. In our expression of the exciton Hamiltonian we have assumed the same values for the conduction- and valence-band mass parameters and the static dielectric constant in GaAs and $Ga_{1-x}Al_xAs$. For most practical quantum-well structures these should be good approximations, since for the most commonly used values of x, these physical parameters are not too different in the two materials.[13] The potential wells for the conduction electron $V_{ew}(z_e)$ and for the holes $V_{hw}(z_h)$ are assumed to be square wells of width L,

$$V_{\rm ew}(z_e)=\begin{cases}0, & |z_e|<L/2\\ V_e, & |z_e|>L/2\end{cases} \tag{3a}$$

and

$$V_{\rm hw}(z_h)=\begin{cases}0, & |z_h|<L/2\\ V_h, & |z_h|>L/2\ .\end{cases} \tag{3b}$$

Here we have chosen, without any loss of generality, the origin of the coordinate system to be the center of the GaAs well. The values of V_e and V_h are determined from the Al concentration in $Ga_{1-x}Al_xAs$ using the following expression for the total energy-band-gap-discontinuity[13]

$$\Delta E_g=1.155x+0.37x^2 \tag{4}$$

in units of electron volts. The values of V_e and V_h are assumed to be 85% and 15% of ΔE_g, respectively.

As pointed out earlier, due to reduction in symmetry along the axis of growth and the presence of energy-band discontinuities, the degeneracy of the valence band of GaAs is removed, leading to the formation of heavy-hole and light-hole excitons. In principle, one would like to solve for the energy levels of these excitons using the full Kohn-Luttinger Hamiltonian which is expressed in terms of a 4×4 matrix,[11] neglecting the split-off valence band. This is a complicated problem to solve. In order to make the problem tractable and to gain some insight into the behavior of these excitons in a magnetic field, we ignore the contribution of the off-diagonal terms (we discuss this point later in this paper) as has been done in all previous calculations in a zero magnetic field. With this approximation the Hamiltonian of an exciton associated with either the heavy-hole or the light-hole band can be expressed as[11]

$$\begin{aligned}H=&-\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right]-\frac{\mu_\pm}{m_e}\frac{\partial^2}{\partial z_e^2}\\&-\frac{\mu_\pm}{m_\pm}\frac{\partial^2}{\partial z_h^2}-\frac{2}{r}+\gamma L_z+\frac{1}{4}\gamma^2\rho^2+V_{\rm ew}(z_e)\\&+V_{\rm hw}(z_h)\ .\end{aligned} \tag{5}$$

Here m_e is the effective mass of the conduction electron, $m_\pm$ is the heavy- (+) or light- (−) hole mass along the z direction, and $\mu_\pm$ is the reduced mass corresponding to heavy- (+) or light- (−) hole bands in the plane perpendicular to the z axis. Both $\mu_\pm$ and $m_\pm$ can be expressed in terms of the well-known Kohn-Luttinger band parameters γ_1 and γ_2 as[11]

$$\frac{1}{\mu_\pm}=\frac{1}{m_e}+\frac{1}{m_0}(\gamma_1\pm\gamma_2) \tag{6}$$

and

$$\frac{1}{m_\pm}=\frac{1}{m_0}(\gamma_1\mp2\gamma_2)\ , \tag{7}$$

where m_0 is the free-electron mass. In these equations the upper sign refers to the $J_z=\pm\frac{3}{2}$ (heavy-hole) band and the lower sign to the $J_z=\pm\frac{1}{2}$ (light-hole) band. The relative electron-hole coordinates in the cylindrical coordinate system are designated by ρ, ϕ, and z. We use a cylindrical gauge and define vector potential $\mathbf{A}$ as

$$\mathbf{A}=\tfrac{1}{2}(\mathbf{B}\times\mathbf{r})\ . \tag{8}$$

The parameter γ is a dimensionless measure of the magnetic field and is defined as

$$\gamma=\frac{e\hbar B}{2\mu_\pm cR}\ , \tag{9}$$

where the effective Rydberg

$$R_\pm=\frac{e^4\mu_\pm}{2\epsilon_0^2\hbar^2}\ . \tag{10}$$

In Eq. (5), L_z is the z component of the angular momentum operator (in units of $\hbar$). Finally it should be noted that the exciton Hamiltonian [Eq. (5)] is in dimensionless form where the energies have been expressed in terms of $R_\pm$ and lengths in terms of effective Bohr radius

$$a_\pm=\frac{\epsilon_0\hbar^2}{\mu_\pm e^2}\ . \tag{11}$$

We have calculated the binding energy of the ground state of the Hamiltonian described by Eq. (5) following a variational approach. For commonly used values of x and L, the barrier heights V_e and V_h are considerably larger than the effective Rydbergs. Thus, the energy associated with the Coulomb interaction will, except for large well widths, be small compared to the electron and hole subband energies in the square well. Because of this, it is helpful to factor explicitly the solutions to the ground state of an electron and a hole in the one-dimensional square well, f_e and f_h, out of the variational wave function ψ

$$\psi=f_e(z_e)f_h(z_h)G(\rho,z,\phi)\ , \tag{12}$$

where $G(\rho,z,\phi)$ describes the internal state of an exciton. For an electron, for instance, the solution of the square-well problem $f_e(z_e)$ can be written as[14]

$$f_e(z_e)=\begin{cases}\cos(k_e z_e), & |z_e|<L/2\\ A_e e^{-\kappa_e|z_e|}, & |z|>L/2\end{cases}. \tag{13}$$

The parameter k_e is determined from the energy of the first subband, and A_e and κ_e are obtained from k_e by requiring continuity of f_e and its first derivative at the interface. The hole wave function f_h is obtained in a similar fashion.

The Hamiltonian of our system [Eq. (5)] has cylindrical symmetry. The z component of the angular momentum is therefore a good quantum number and the ϕ dependence of the wave function thus has the form $e^{im\phi}$, where m is an integer. In addition, the Hamiltonian is also invariant under reflections through the origin. The wave function therefore has a definite parity. In view of this knowledge, the function $G(\rho,z,\phi)$ can be written in the form

$$G(\rho,z,\phi)=\rho^{|m|}e^{im\phi}\sum_{i,j}A_{ij}G_{ij}(\rho,z)\ . \tag{14}$$

The basis functions $G_{ij}(\rho,z)$ are taken to be the products of Gaussians in ρ and z variables:

$$G_{ij}(\rho,z)=e^{-\alpha_i z^2}e^{-(\alpha_j+\beta)\rho^2}\ . \tag{15}$$

This choice is made because of the success of a similar basis set which Aldrich and Greene[15] used to solve the problem of a hydrogen atom in a magnetic field. They found that the use of Gaussian basis sets yielded good results for the ground and several excited states throughout the range $0<\gamma<10$. The set of parameters α_i used in this work are taken from the results of Huzinaga[16] who performed a detailed study of the use of Gaussian basis functions in the calculations of the energy levels of a hydrogen atom. This set of α_i gives energies of $1s$, $2s$, and $2p$ free-hydrogen atom states accurate to within 0.001 Ry. The parameter β was varied in each case to minimize the energy and is primarily determined by the value of the magnetic field.

The energies are obtained by solving the following equation:

$$\det(\underline{H}-E\underline{U})=0\ , \tag{16}$$

where $\underline{H}$ and $\underline{U}$ are the Hamiltonian and overlap matrices, respectively. For computational reasons we restrict the basis functions by requiring $A_{ij}=0$ for $|i-j|>0$. This has little effect on the energies obtained. The number of basis functions used (and hence the order of the Hamiltonian and overlap matrices) in our calculation is 5. The binding energy of the ground state E_B is then given as

$$E_B=E_e+E_h+\gamma-E\ , \tag{17}$$

where E_e and E_h are the lowest subband energies of the electron and the hole, respectively, γ is the energy of the first Landau level,[15] and E is the eigenvalue of the Hamiltonian [Eq. (5)] corresponding to the $1S$ level, which has been determined variationally. The values of E_e and E_h are obtained by numerically solving the following transcendental equations:[14]

$$\left[\frac{E_e}{V_e}\right]^{1/2}=\cos\left[\left[\frac{m_e E_e}{2\hbar^2}\right]^{1/2}L\right] \tag{18a}$$

and

$$\left[\frac{E_h}{V_h}\right]^{1/2}=\cos\left[\left[\frac{m_{\pm}E_h}{2\hbar^2}\right]^{1/2}L\right]\ . \tag{18b}$$

This procedure results in our variational binding energies being rigorous lower bounds for the true binding energies.

RESULTS AND DISCUSSION

We have calculated the values of the binding energies (E_B) of the heavy-hole exciton and the light-hole exciton as a function of L for several values of the magnetic field using finite potential barriers. The values of the various physical parameters pertaining to GaAs (Ref. 7) used in our calculations are $m_e=0.067m_0$, $\epsilon_0=12.5$, $\gamma_1=7.36$ and $\gamma_2=2.57$. The values of the heavy-hole mass (m_+) and the light-hole mass (m_-) obtained using these values of γ_1 and γ_2 are $0.45m_0$ and $0.08m_0$, respectively. The reduced mass in the x-y plane for the heavy-hole ($J_z=\pm\frac{3}{2}$) exciton (μ_+) is $0.04m_0$ and the light-hole ($J_z=\pm\frac{1}{2}$) exciton (μ_-) is $0.051m_0$. The value of μ_+ is less than that of μ_- due to the anisotropic nature of the kinetic energy expressions in the diagonal terms of the Kohn-Luttinger Hamiltonian of an exciton.[11]

In Fig. 1 we display the variation of E_B of a heavy-hole exciton as a function of L for several different values of the magnetic field, for a commonly used value of Al concentration $x=0.3$. Similar results for the light-hole exciton are displayed in Fig. 2. For comparison, we also show the variation of E_B with L for zero magnetic field. There are several interesting features to be noted in these plots.

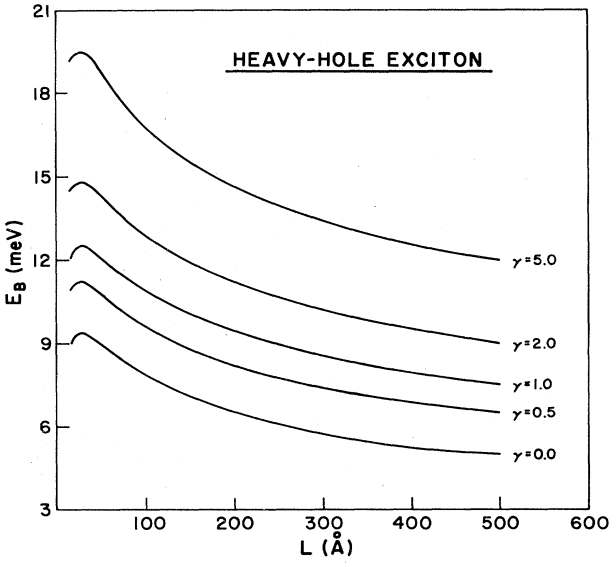

FIG. 1. Variation of the binding energy of the ground state (E_B) of a heavy-hole exciton as a function of the well size (L) for Al concentration $x=0.3$. Five different values of the magnetic field parameter γ (defined in the text) are shown.

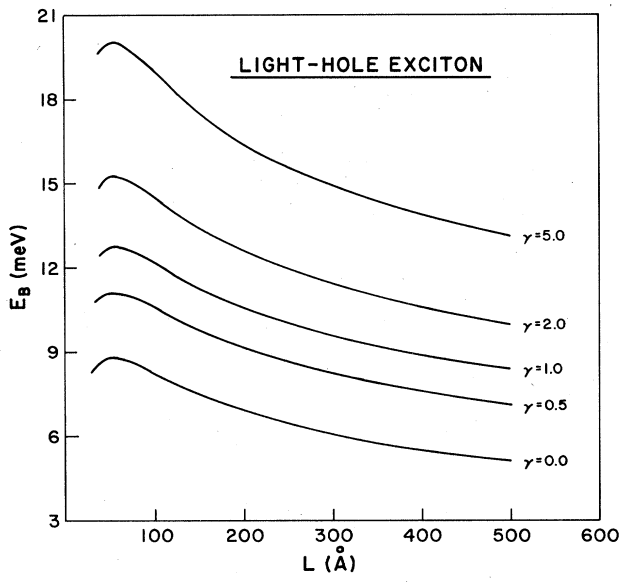

FIG. 2. Variation of the binding energy of the ground state (E_B) of a light-hole exciton as a function of the well size (L) for Al concentration $x=0.3$. Five different values of the magnetic field parameter γ (defined in the text) are shown.

As expected, the presence of a magnetic field leads to more binding. The value of E_B, both for the heavy-hole exciton and for the light-hole exciton, increases as L is reduced until it reaches a maximum and then decreases quite rapidly. The value of L at which E_B reaches a maximum (L_c) is larger for the light-hole exciton. The reason for this behavior of E_B is quite simple and has been discussed elsewhere.[5,7] For a given value of x and for a given exciton system, the value of L_c is about the same for all values of the magnetic field. In addition we find that the separation between curves of different values of γ increases as L decreases. This happens because at smaller well widths the extension of the wave function in the x-y plane is reduced. This decreases the contribution of the magnetic term of the Hamiltonian [Eq. (5)] which is proportional to ρ^2. A reduction of this positive term leads to an increase in the binding energy.

As noted earlier, we have assumed the conduction-band discontinuity to be 85% of the total band-gap difference. It has recently been suggested that 57% may be a more appropriate value.[17] For a given value of Al concentration, the binding energies of both the heavy-hole exciton and the light-hole exciton are found to be relatively insensitive to this suggested change in the barrier height.

Several groups[1–3,9,10] have attempted to measure the values of the binding energies of these two exciton systems in GaAs-$Ga_{1-x}Al_xAs$ quantum well structures in recent years. Recently Maan *et al.*[9] and Miura *et al.*[10] have studied the behavior of these excitons in GaAs-$Ga_{1-x}Al_xAs$ quantum well systems as a function of L in the presence of high magnetic fields (≤ 230 kG) using excitation spectroscopic and absorption techniques, respectively. At zero magnetic field both Maan *et al.*[9] and Miura *et al.*[10] find that the values of the binding energies of both the heavy-hole exciton and the light-hole exciton they measure are considerably larger than those determined by Miller *et al.*[3] For instance, the value of E_B for the heavy-hole exciton for the 50-Å well they measure is about 17 meV as compared to 12 meV determined by Miller *et al.*[3] Similar results are found for the other well sizes. In addition, they also find that the values of E_B for the heavy-hole exciton are always larger than those of the light-hole exciton, a result contrary to that of Miller *et al.*[3] and to our result. The reasons for the difference between the experimental results of Miller *et al.*[3] and those of Maan *et al.*[9] and Miura *et al.*[10] are not clear.

The values of E_B for the excitons in a zero magnetic field that we calculate, are considerably smaller than those measured in Refs. 9 and 10. Maan *et al.*[9] have also derived the reduced exciton masses from their measurements of Landau levels and find that these are considerably larger than those in bulk GaAs, namely, the values we have used. For instance, the reduced mass of the heavy-hole exciton varies from $0.069m_0$ to $0.084m_0$ for well sizes 125 to 50 Å. When we use these values in our calculations we find that our results agree rather well with the experimental values of the binding energies. Maan *et al.*[9] and Miura *et al.*[10] have studied the variation of binding energies with magnetic field up to fields of 230 kG. Our results agree qualitatively with the observed variation. However, if we use the larger reduced masses in our calculations the theoretical results agree very well with the experimental values. Recently several groups[18–20] have examined the dispersion relations of free holes in a quantum well using the Kohn-Luttinger Hamiltonian. They find that for finite values of wave vectors in the x-y plane there is a considerable mixing of light- and heavy-hole bands leading to strong nonparabolicities. It appears that to get a good quantitative agreement between theory and experiment one really needs to solve the problem of excitons in a quantum well in a magnetic field using the full Kohn-Luttinger Hamiltonian and thus take into account properly the interband mixing. This, as mentioned earlier, is a complicated problem to solve. Our approach in which we treat the valence-band structure in terms of two decoupled bands is primarily intended to provide an insight into the behavior of these excitons in a magnetic field.

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