Exciton binding energy in a quantum well with inclusion of valence-band coupling and nonparabolicity

U. Ekenberg
Department of Theoretical Physics, 1 Keble Road, Oxford OX1 3NP, United Kingdom

M. Altarelli
Max-Planck-Institut für Festkörperforschung, Hochfeld-Magnetlabor, 166 X, F-38042 Grenoble Cedex, France

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Binding energies of excitons associated with several transitions between different subbands in undoped quantum wells are calculated for different well widths using a novel perturbational approach. The degeneracy of the valence band, the nonparabolicity of the conduction band, and the matching of the wave function at the interfaces are taken into account. The zeroth-order wave function is taken to be the product of the envelope functions in the z direction (perpendicular to the layers) for the electron and the hole and a purely two-dimensional (2D) exciton wave function. The difference between the 2D and 3D interaction between the electron and the hole is included in a variational-perturbational approach. The effect of the valence-band degeneracy on the properties of the holes is described with the use of the 4×4 Luttinger Hamiltonian. We include the off-diagonal elements of this matrix in perturbation theory up to second order. This involves summations over the bound exciton states and integrals over the continuum states, which are found to be important. These off-diagonal elements in some cases modify the results considerably and improve the agreement with recent experimental results.

I. INTRODUCTION

GaAs-$Al_xGa_{1-x}As$ quantum wells have been extensively investigated by optical experiments during the last years. In this system both the electrons and the holes are largely confined to the GaAs layer. The optical spectra are often dominated by excitonic transitions from hole subbands below the bulk valence-band edge to electron subbands above the conduction-band edge. For an accurate interpretation of these experiments a good knowledge of the exciton binding energies is essential.

Many calculations of exciton binding energies in quantum wells have been performed in the last years.[1-12] Most of these calculations[1-8] have treated the hole as a particle with either the heavy-hole or the light-hole mass. However, an accurate description of the exciton should take the degeneracy of the valence band in the bulk into account. While this only gives a small correction for bulk excitons,[13] it has been shown[14,9] that this has a large effect on the hole subband dispersion parallel to the layers. These subbands are strongly nonparabolic and some subbands even have maxima at $k\neq0$, i.e., they have electron-like masses near $k=0$. The density of states is far from the steplike function, which results from parabolic subbands, and the $k\neq0$ maxima correspond to sharp peaks in the density of states in the valence band and also in the joint density of states.[14]

It should not be surprising that these strong anomalies also can influence the exciton properties substantially. The fourfold degeneracy (including spin) of the top of the valence band is accurately described by a 4×4 matrix, usually called the Luttinger Hamiltonian.[15,16] The main purpose of this paper is to investigate the effect of the off-diagonal elements of this matrix which couple the heavy-hole and light-hole subbands. The split-off band is in GaAs 0.34 eV below the valence-band edge[17] and is therefore neglected.

Some variational calculations which include the coupling between the hole subbands have recently been performed.[9-12] We have instead chosen a novel perturbational approach, which directly displays the effect of the off-diagonal elements in the Luttinger Hamiltonian. We choose our zeroth-order wave function to be a product of the envelope functions for the electron and the hole in the z direction (perpendicular to the layers) and a purely two-dimensional (2D) exciton. The difference between the three-dimensional (3D) and 2D interaction between the electron and the hole is treated using a variational-perturbational approach.[5] Finally the off-diagonal elements of the Luttinger Hamiltonian are included in perturbation theory up to second order. The effect of the conduction-band nonparabolicity is also considered. Explicit expressions for the matrix elements are presented and the numerical work is reduced to evaluating sums and integrals and solving transcendental equations to find the sublevels.

We describe the theory in Sec. II and present the results in Sec. III. A comparison with experimental and other theoretical results and a discussion follow in Sec. IV, the conclusions are given in Sec. V, and some mathematical details are given in the Appendix.

II. THEORY

We treat the exciton in the effective-mass approximation[18,16] and write the Hamiltonian

$$H=-\frac{\hbar^2}{2m_e}\nabla_e^2+T_h(-i\nabla_h)+V_e(z_e)+V_h(z_h) -\frac{e^2}{\epsilon|\mathbf{r}_e-\mathbf{r}_h|}\ . \tag{1}$$

Here the first term is the kinetic energy of an electron with effective mass m_e while the second term, which will be explained below, gives the kinetic energy of the hole. The next two terms describe the confinement potentials for the electron and the hole, respectively. We take them to be finite square-well potentials:

$$V_{e(h)}(z)=0, \quad |z|<b \tag{2}$$

$$V_{e(h)}(z)=\Delta E_{c(v)}, \quad |z|>b\ . \tag{3}$$

Here $2b$ is the width of the well while ΔE_c (ΔE_v) is the conduction- (valence-) band discontinuity at the GaAs-$Al_xGa_{1-x}As$ interface for electrons and holes, respectively. The last term in Eq. (1) describes the Coulomb interaction between the electron and the hole with ϵ being the static dielectric constant. The exciton binding energies are given by the difference of the eigenvalues of the Hamiltonian with and without this term.

$T_h(\mathbf{k})$ is the Luttinger matrix[15] which describes the dispersion of the valence band. One convenient representation is

$$T_h(\mathbf{k})=\begin{pmatrix} A_+ & B & C & 0 \\ B^* & A_- & 0 & C \\ C^* & 0 & A_- & -B \\ 0 & C^* & -B^* & A_+ \end{pmatrix}, \tag{4}$$

where

$$A_\pm=\frac{\hbar^2}{2m_0}[(\gamma_1\pm\gamma_2)(k_x^2+k_y^2)+(\gamma_1\mp2\gamma_2)k_z^2]\ , \tag{5}$$

$$B=-\frac{\hbar^2}{m_0}\sqrt{3}\gamma_3k_z(k_x-ik_y)\ , \tag{6}$$

and

$$C=-\frac{\hbar^2}{2m_0}\sqrt{3}[\gamma_2(k_x^2-k_y^2)-2i\gamma_3k_xk_y]\ . \tag{7}$$

The valence-band structure is thus described by three material parameters γ_1, γ_2, and γ_3, which are related to inverse effective masses. The heavy-hole mass in the k_z direction is given by $m_h=(\gamma_1-2\gamma_2)^{-1}$ (in units of the free-electron mass, m_0, which we henceforth set equal to one) while the light-hole mass is $m_l=(\gamma_1+2\gamma_2)^{-1}$. In some earlier calculations of excitons in quantum wells[1,3,5,6] the coefficients along the diagonal in Eq. (4) in front of $k_x^2+k_y^2$ have been interpreted as "transverse masses." This implies that the "light-hole" mass, $(\gamma_1-\gamma_2)^{-1}$, becomes heavier than the "heavy-hole" mass, $(\gamma_1+\gamma_2)^{-1}$. Ignoring the off-diagonal elements of the matrix (4) in this way simplifies the exciton calculation considerably, but it is dubious. The coupling between the hole subbands influences the subband dispersion in a 2D system strongly[14,9] and it will be shown below that these off-diagonal elements also give important corrections to the exciton binding energies.

We follow the effective-mass-theory prescription[16,18] and use this matrix to represent the kinetic energy of the hole with the replacement $\mathbf{k}\rightarrow-i\nabla$. In the calculation of bulk excitons the electron and hole coordinates are replaced by their relative coordinates and suitable coordinates which describe the motion of the whole exciton. In the present case the confinement potentials apply to the z coordinate of the electron and the hole separately, not their relative coordinate. Therefore it turns out to be convenient to keep the z coordinates z_e and z_h and introduce their relative coordinates x and y [or $\rho=(x^2+y^2)^{1/2}$ and $\phi=\tan^{-1}(y/x)$] in the plane parallel to the interfaces. We take $K_{||}$, which describes the motion of the whole exciton in this plane, to be zero.

While the heavy-hole and light-hole bands are degenerate at $k=0$ in the bulk, this degeneracy is lifted in a quantum well, where a set of heavy-hole levels and a set of light-hole levels are formed. This lifting of the degeneracy is a strong effect, which hardly can be treated as a perturbation. We have therefore included the confinement of the electron and the hole in the zeroth-order Hamiltonian. To make the perturbation treatment tractable we also include the Hamiltonian of a purely 2D exciton in the zeroth-order Hamiltonian. The total Hamiltonian is rewritten

$$H=H_0^e+H_0^h+H_0^{\rm exc}+H_1+H_2\ , \tag{8}$$

where

$$H_0^e(z_e)=-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2}+V_e(z_e)\ , \tag{9}$$

$$H_0^h(z_h)=-\frac{\hbar^2}{2}(\gamma_1\mp2\gamma_2)\frac{\partial^2}{\partial z_h^2}+V_h(z_h)\ , \tag{10}$$

$$H_0^{\rm exc}(\rho)=-\frac{\hbar^2}{2}\left[\frac{1}{m_e}+\gamma_1\pm\gamma_2\right]\times\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]-\frac{\lambda e^2}{\epsilon\rho}\ , \tag{11}$$

$$H_1(z_e,z_h,\rho)=\frac{\lambda e^2}{\epsilon\rho}-\frac{e^2}{\epsilon[\rho^2+(z_e-z_h)^2]^{1/2}}\ , \tag{12}$$

and

$$H_2(z_h,x,y)=\begin{pmatrix} 0 & B & C & 0 \\ B^* & 0 & 0 & C \\ C^* & 0 & 0 & -B \\ 0 & C^* & -B^* & 0 \end{pmatrix}, \tag{13}$$

where

$$B=\hbar^2\sqrt{3}\gamma_3\frac{\partial}{\partial z_h}\left[\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right] \tag{14}$$

and

$$C=\hbar^2\frac{\sqrt{3}}{2}\left[\gamma_2\left[\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}\right]-2i\gamma_3\frac{\partial^2}{\partial x\,\partial y}\right]\ . \tag{15}$$

In Eqs. (10) and (11) the upper (lower) sign corresponds to heavy-hole (light-hole) excitons. The first three terms in Eq. (8) are included in the zeroth-order Hamiltonian. The zeroth-order wave function is separable and can be written

$$\psi_0 = \psi_0^e(z_e)\psi_0^h(z_h)\psi_0^{\rm exc}(\rho,\phi) \ . \tag{16}$$

We have added and subtracted the term $\lambda e^2/\epsilon\rho$, which corresponds to the component of the electron-hole interaction in the x-y plane. This idea was introduced by Lee, Mei, and Liu[19] and subsequently used by Jiang[5] in solving the exciton problem. If we treated the term H_1 exactly, the total energy should not depend on the choice of the parameter λ, which only determines how the energy is divided between H_0 and H_1. We can therefore choose λ to minimize the expectation value of H_1. We make the approximation to treat H_1 in first-order perturbation theory only. We can always choose $\langle H_1 \rangle$ to be zero. Physically this means that the effective potential

$$V(\rho) = -\int\int dz_e dz_h [\psi_0^e(z_e)]^2[\psi_0^h(z_h)]^2 \times \frac{e^2}{\epsilon[\rho^2+(z_e-z_h)^2]^{1/2}} \tag{17}$$

used by various authors[20,6,9,10] is replaced by a 2D potential, which is scaled down so that the expectation values of the two potentials are equal.

In this way the matrix elements of H_2, the off-diagonal elements of the Luttinger Hamiltonian, can be performed analytically. It is seen from parity considerations that the first-order contribution from H_2 vanishes. We must therefore resort to second-order perturbation theory and evaluate the matrix elements between the state we want to calculate and all other eigenstates of H_0. The reason why H_2 is treated as a perturbation is that it contains γ_2 and γ_3 which are one order of magnitude smaller than the coefficients of the diagonal terms, which contain $m_e^{-1}+\gamma_1 \approx 22$.

The envelope wave functions ψ_0^e and ψ_0^h are easily obtained. They can be divided into two groups with even and odd parity, respectively. We apply the usual boundary conditions that the envelope function and its derivative divided by the effective mass should be continuous across the interfaces. This leads to simple transcendental equations from which the energies are obtained numerically. $H_0^{\rm exc}(\rho)$ is equivalent to the Hamiltonian for a 2D hydrogen atom. The 2D exciton problem has been treated by Ralph[21] and by Shinada and Sugano[22] and the analytic solutions for both bound states and continuum states have been given in Ref. 22.

The first term of the matrix element of H_1 is easily evaluated. For the second term the ρ integral can be performed analytically. The result can be expressed in terms of Struve and Neumann functions. We have, however, evaluated the whole triple integral numerically.

To evaluate the second-order correction we are to sum over bound states and integrate over continuum states. It can be seen from Eq. (13) that the heavy-hole states always couple to light-hole states and not to other heavy-hole states. From parity considerations it is clear that the sum over matrix elements of the term B [Eq. (14)] is over quantum-well states of the opposite parity while for the C-term we have to sum over states with the same parity. The matrix elements can be separated into integrals over z_e, z_h, and ρ. The ρ integrals can be performed analytically both for bound states and continuum states although the evaluation is quite laborious. The mathematical details are found in the Appendix. In some cases we have to integrate over energies of continuum states which coincide with the state whose energy we want to compute. In order to simulate the lifetime broadening of these exciton states we have added a small imaginary part to the energy denominator in the second-order perturbation expression. The effect of these Fano resonances[23] will be investigated in more detail later.

The z integrals are also evaluated analytically. In addition to summing over the bound quantum-well states we should integrate over the continuum states. For normalization purposes we apply the boundary conditions that the continuum wave functions vanish at $\pm L$, where L is chosen to be much larger than the well width (cf. Ref. 24). This implies that we actually sum over a large number of densely spaced states. If L is large enough it turns out that the results are quite insensitive to L.

III. RESULTS

If the GaAs layers are not very thin, there are several electron subbands above the bulk conduction-band edge, which we label En, $n=1,2,3,\ldots$. Similarly we have heavy-hole subbands Hn and light-hole subbands Ln below the bulk valence-band edge. The strongest peaks in the optical spectra usually follow the selection rule $\Delta n=0$. However, transitions with $\Delta n \neq 0$ have also been observed[25] and theoretically explained[9] in terms of mixing of heavy-hole and light-hole character of the hole subbands for finite values of the wave vector parallel to the layers. For each transition between a hole subband and an electron subband the exciton binding energy E_B is in general different.

The input parameters are given in Table I. For $Al_xGa_{1-x}As$ we use linear interpolation between the parameters for GaAs and AlAs. The valence-band discontinuity is taken to be 35% of the band-gap difference between GaAs and $Al_xGa_{1-x}As$, for which we use the expression $1.247x$ eV (Ref. 27).

In Fig. 1 we show the 1s (ground-state) exciton binding energies as a function of GaAs well width for the transitions H1→E1 and L1→E1, which are usually the most prominent features in the optical spectra. The barriers are here taken to consist of $Al_{0.4}Ga_{0.6}As$. It is seen that E_B is enhanced by a factor of 2–3 over the bulk value 4.4 meV

TABLE I. Parameters used in the calculations. From Ref. 26.

		GaAs	AlAs
Electron mass m_e		0.0665	0.15
Valence-band parameters:	γ_1	6.85	3.45
	γ_2	2.1	0.68
	γ_3	2.9	1.29
Dielectric constant	ϵ	12.56	(not used)

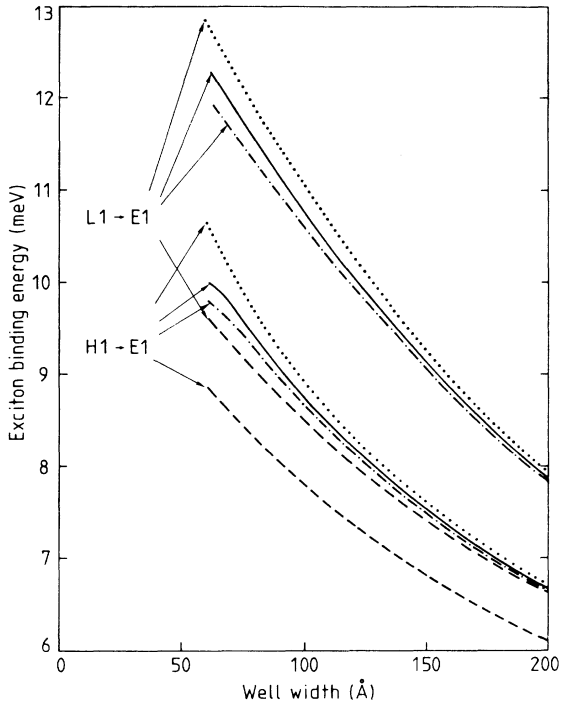

FIG. 1. Exciton binding energy versus width of the GaAs well for transitions from heavy-hole level 1 (H1) and light-hole level 1 (L1) to electron level 1 (E1). The dashed lines are the result without H_2 [the off-diagonal elements in the matrix (4)] while the dashed-dotted lines are with H_2 included in second-order perturbation theory. The solid lines show the effect when the conduction-band nonparabolicity according to Eq. (20) is included in addition to H_2, while the dotted lines show the effect when Eq. (21) is used to define the effective mass for motion parallel to the layers. The barriers consist of $Al_{0.4}Ga_{0.6}As$.

(Ref. 13) and that it increases with decreasing well width down to about 60 Å. In the limit $b \to 0$ it should decrease again towards the value for bulk $Al_{0.4}Ga_{0.6}As$. However, for very thin layers the use of the effective-mass approximation is dubious and we have therefore not included any results for well widths smaller than 60 Å.

We have separately shown the result with and without the off-diagonal elements in the Luttinger Hamiltonian [H_2 in Eq. (13)] included. We see that these elements have a clear effect and enhance the H1→E1 and L1→E1 binding energies by about 1 and 2 meV, respectively. This enhancement increases somewhat with decreasing well width. The fact that E_B for the L1→E1 transition is particularly strongly enhanced is thought to be related to the anomalous dispersion of the L1 subband.[9,14] In fact, all the binding energies of excitons related to L1 and H3, which also has anomalous dispersion, are strongly enhanced.

For relatively thin wells the subbands are fairly far from the bulk band edge and the use of a parabolic dispersion becomes inaccurate. A convenient way to include the effect of band nonparabolicity is to express it in terms of an energy-dependent effective mass. A commonly used expression for the electron mass was derived by Kolbas.[28,29] It is actually an optical mass derived from a three-band Kane model[30,31] evaluated at 77 K. An accurate expression for the bulk conduction-band dispersion at $T=0$ was recently derived by Braun and Rössler[32] using a five-band (14-band if the degeneracies at $k=0$ are included) $\mathbf{k}\cdot\mathbf{p}$ theory:

$$E(\mathbf{k})=\frac{\hbar^2}{2m}k^2+\alpha_0 k^4+\beta_0(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2) \pm\gamma_0[k^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)-9k_x^2k_y^2k_z^2]^{1/2} , \tag{18}$$

where $m=0.0665m_0$, $\alpha_0=-1.969\times10^{-29}$ eV cm^4, $\beta_0=-2.306\times10^{-29}$ eV cm^4 and $\gamma_0=-2.8\times10^{-23}$ eV cm^3 for GaAs. The last term represents the spin splitting and vanishes in the [001] and [111] directions. The expression for the dispersion in the [001] direction can be rewritten

$$E(k)=\frac{\hbar^2k^2}{2m}\left[1-\alpha'\frac{\hbar^2k^2}{2m}\right] , \tag{19}$$

where $\alpha'=0.60$ eV^{-1}. If we invert Eq. (19) we find to lowest order

$$\hbar^2k^2\simeq 2Em(1+\alpha'E) , \tag{20}$$

where $m^*=m(1+\alpha'E)$ can be taken as an energy-dependent effective mass.[33] It is not difficult to insert this expression into the transcendental equations (A5), which give the subband energies E_i. The simplest approximation is to use the corresponding effective masses m_i^* also for the effective Bohr radius of the 2D exciton in Eq. (A14b). These results are given by the solid line in Fig. 1. A better approximation is to neglect the spin-splitting, take the solution of Eqs. (A5) with Eq. (20) (for $k_{\|}=0$) as the zeroth-order wave function and treat the mixed term in Eq. (18) $(2\alpha_0+\beta_0)k_z^2(k_x^2+k_y^2)$ in first-order perturbation theory. Nonparabolicity effects in $Al_xGa_{1-x}As$ are ignored. Then the coefficient in front of the $(k_x^2+k_y^2)$ becomes

$$\frac{\hbar^2}{2m}+(2\alpha_0+\beta_0)\frac{k^2b+\frac{1}{2}tk\sin(2kb)}{b+\frac{t\sin(2kb)}{2k}+\frac{1+t\cos(2kb)}{2s}} , \tag{21}$$

where $s=[2m_2(V-E)]^{1/2}/\hbar$, $t=+1$ ($t=-1$) for states with even (odd) parity and k is given by Eq. (20). (V is here the conduction-band discontinuity and m_2 is the effective mass in $Al_xGa_{1-x}As$.) This expression can be used to define an energy-dependent effective mass for the motion parallel to the layers.[34] If this mass is used in Eq. (A14b) for the 2D exciton, the nonparabolicity effects are much stronger, as is shown by the dotted line in Fig. 1.

Recent experiments[35] indeed indicate that the nonparabolicity can be quite different for motion perpendicular to and parallel to the quantum well and that it can be much stronger than the bulk value in the latter case. The bulk heavy-hole band is parabolic to a good approximation. But the nonparabolicity of the light-hole subband should also be considered in a more accurate treatment. An

TABLE II. Exciton binding energies in meV for several transitions from heavy-hole (Hn) and light-hole (Ln) levels to electron levels (En). The result without inclusion of H_2 is given in parentheses. The well width is 150 Å and the barriers consist of $Al_{0.4}Ga_{0.6}As$. The levels E4, H6, H7, and L4 are also bound but the results are not included here for reasons discussed in the text.

	Electron levels		
Hole levels	E1	E2	E3
H1	7.5 (6.8)	6.4 (5.8)	6.3 (5.8)
H2	9.4 (6.0)	9.2 (5.8)	8.9 (5.5)
H3	8.6 (6.0)	8.2 (5.6)	8.1 (5.6)
H4	8.4 (5.9)	7.9 (5.6)	7.8 (5.5)
H5	8.0 (5.9)	7.6 (5.6)	7.5 (5.5)
L1	9.1 (7.4)	7.8 (6.4)	7.7 (6.3)
L2	3.9 (6.3)	3.9 (6.3)	3.7 (6.0)
L3	3.9 (6.1)	3.7 (5.9)	3.7 (5.9)

energy-dependent effective light-hole mass can for example be derived from the work of Schuurmans and 't Hooft.[36]

In Table II we give the exciton binding energies for different transitions and fixed well size. For transitions from a given hole level E_B becomes somewhat smaller for excited electron levels than for the ground state. This effect is not difficult to explain qualitatively: the higher electron states correspond to wave functions which penetrate more into the barriers. The electrons are therefore less confined to the GaAs well and the overlap with the hole wave function is smaller. The differences in E_B are small between the different excited electron states and the trends seen in Table II are sometimes changed when the effect of conduction-band nonparabolicity is included.

We see a similar trend for transitions from different hole levels to a given electron level if H_2 in Eq. (13) is neglected. But the effect of H_2 is quite different for different transitions and overshadows this trend. For most transitions the exciton binding energy is enhanced by an amount which depends on the position of the other hole subbands with which the hole subband of interest is coupled. For transitions from some hole levels (e.g., L2 and L3 in Table II) H_2 gives a negative correction because of the interaction with more strongly bound heavy-hole states. It should be noted that the levels L1 and H2 are very close to each other for the parameters we have used. The results for excitons involving these levels could be significantly different if, e.g., other valence-band parameters were used.

Concerning the contribution of the different types of second-order terms to E_B the matrix elements of B [Eq. (14)] are generally much larger than those of C [Eq. (15)]. Thus heavy-hole states are more strongly coupled to the light-hole states of the opposite parity than to those of the same parity. There is, e.g., strong coupling between L1 and H2. This is of importance of the oscillator strengths of normally "forbidden" transitions. The H2 p state [$m=1$ in Eq. (A13)] can, e.g., gain oscillator strength from the L1 s state.[10] A double peak for the H2→E1 excitonic transition has recently been observed in experiments with an electric field perpendicular to the layers.[37] These peaks can possibly be due to $1s$ and $2p$ excitons.

It is interesting that the continuum exciton states usually give a larger contribution than the bound states. The continuum states of the quantum well give a negligible contribution to E_B for the lowest hole states. But the contribution is more than a meV for transitions from some excited hole states, e.g., H4 and H5 for a well width of 150 Å (Table II).

IV. DISCUSSION

The results of this calculation are thought to be most reliable for intermediate layer thicknesses. As was mentioned above the effective-mass approximation becomes inaccurate for very thin layers. Then the energy levels are also fairly far from the bulk band edges and the nonparabolicity is stronger. It is then also dubious to use GaAs parameters for the purely 2D exciton since they ought to be influenced by the $Al_xGa_{1-x}As$ parameters for states with wave functions penetrating substantially into the barriers. On the other hand, the zeroth-order Hamiltonian contains a pure 2D electron-hole interaction. Although the correct 3D interaction is included as a perturbation, the matrix elements of H_2 are evaluated with this 2D potential and the results can be expected to be less accurate when the GaAs layer becomes thick and the 3D limit is approached. An analogy with the two variational functions used in Ref. 2 suggests that our results should be reliable up to a well width of about 200 Å.

The calculations would have been simplified if the barriers were taken to be infinite. We have also done such calculations and found that E_B is then much more enhanced by H_2. This is especially true for transitions from the levels L1 and H3.

An alternative approach would be to include the terms $\pm\gamma_2(k_x^2+k_y^2)$ along the diagonal in Eq. (4) in first- and second-order perturbation theory instead of including them in the zeroth-order Hamiltonian. This approach would be more similar to that for bulk excitons by Baldereschi and Lipari.[13] We have found that this gives E_B values which usually only differ from the results presented here by a few tenths of a meV.

It is not trivial to measure E_B experimentally with high accuracy. Comparing the exciton peaks with the calculated subband energies[38] is an uncertain method since the position of a subband is quite sensitive to the layer width $2b$. (For an infinite well $E \propto b^{-2}$.) Some early experiments[1]

TABLE III. Comparison with experimental results.

Well width (Å)	x	Hole level	Reference	E_B (meV)	Our result[a] (meV)
75	0.4	H1	39	10.5–11.5[b]	9.4
		L1		11.3–12.3[b]	11.4
92	0.35	H1		9.5–10.5[b]	8.8
		L1		11.2–12.2[b]	10.9
100	0.29	H1	40	13	8.5
		L1		10	10.2
112	0.3	H1	41	12	8.2
75	0.35	H1	42	12[c]	9.3
				10[d]	9.3
		L1		11[d]	11.0
110	0.35	H1		9.5[c]	8.4
				8[d]	8.4
		L1		9[d]	9.9

[a]Without conduction-band nonparabolicity.
[b]The limits correspond to an estimate 1–2 meV for the binding energy of the $2s$ exciton, which here is added to the experimentally determined difference between the $1s$ and $2s$ exciton.
[c]High-field extrapolation (see text).
[d]Low-field extrapolation.

assigned a weak shoulder to a $2s$ exciton state, but this can also be interpreted as the onset of the continuum states.[3] The estimated $1s$ binding energy is higher than in our calculation if we use the former interpretation but lower if we use the latter. Dawson *et al.*[39] have recently observed a clearly resolved peak, which is interpreted as a $2s$ exciton. It is straightforward to calculate E_B for $2s$ excitons with the present method, but we have not done this yet. It can be estimated to be 1–2 meV. As is shown in Table III adding this to the experimentally determined $E_B(1s)-E_B(2s)$ tends to give higher values than obtained in this calculation. For the H1→E1 transition the measured $E_B(1s)-E_B(2s)$ actually rather agrees with the calculated $E_B(1s)$.

Several attempts to determine E_B have been made using magneto-optical experiments.[40–42] In Refs. 40 and 41 extrapolations to $B=0$ from high magnetic fields were done. This usually resulted in much higher exciton binding energies than obtained in this calculation. Recent results[42] also include extrapolations from lower magnetic fields. These results are expected to be more reliable and also give clearly lower E_B values. As is seen in Table III the agreement between these results and our calculation is quite good, seldom in disagreement by more than 1 meV. Actually, a more recent fit of the high-field results with nonparabolicity effects taken more carefully into account gives quite good agreement with the low-field results.[43] More experiments are desirable to determine the accuracy of the different calculations.

Many calculations ignoring H_2 but taking the depth of the wells to be finite have been performed.[3,5–7] The results of these calculations usually differ from each other by a few tenths of a meV. Brum and Bastard[7] have also calculated E_B for transitions between higher subbands. Our results without H_2 agree fairly well with theirs for all transitions and are typically some tenths of a meV smaller.

If we compare our results with the variational calculations where the coupling between heavy and light holes has been included,[9–12] we find a good agreement with the calculations by Chan[10] and by Bauer and Ando[12] while Sanders and Chang[9] and Broido and Sham[11] find exciton binding energies more strongly enhanced. The reason for the disagreement with Ref. 11 is possibly that the Coulomb interaction is evaluated for an infinite quantum well of a somewhat larger width than the actual width. In the parabolic approximation this gives higher E_B values than in comparable variational calculations. The reason for the discrepancy between our calculation and Ref. 9 is not quite clear. Since the perturbation in some cases is quite substantial it is conceivable that our perturbation approach in these cases is insufficient and that higher-order terms may be important.

V. CONCLUSIONS

We have calculated exciton binding energies for transitions between several hole and electron subbands in GaAs quantum wells between $Al_xGa_{1-x}As$ layers. The main purpose of the calculation has been to evaluate the effect of the off-diagonal elements of the hole Hamiltonian,[15] which are related to the degeneracy of the bulk valence band. We have found that they give important corrections, which are different for transitions involving different hole subbands and seem to be related to the dispersion parallel to the interfaces for these hole subbands. The exciton binding energies for the transitions H1→E1 and L1→E1 are enhanced by about 1 and 2 meV, respectively, by the off-diagonal elements for typical well sizes. Our results agree quite well with some of the recent experiments[42,43] and theories.[10,12]

Note added in proof. Our results agree well with some recent experiments by A. Petrou, G. Waytena, X. Liu, J. Ralston, and G. Wicks [Phys. Rev. B **34**, 7436 (1986)].

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APPENDIX: EVALUATION OF SECOND-ORDER MATRIX ELEMENTS

The eigenfunctions of the zeroth-order Hamiltonian can be written

$$|i,j,l,n,m\rangle = |i\rangle\,|j\rangle\,|l\rangle\,|n,m\rangle\ , \tag{A1}$$

where $|i\rangle$ are the column vectors $(\delta_{1i},\delta_{2i},\delta_{3i},\delta_{4i})$, $|j\rangle$ are the eigenfunctions of H_0^h, $|l\rangle$ are the eigenfunctions of H_0^e, and $|n,m\rangle$ are the eigenfunctions of $H_0^{\rm exc}$. For continuum states n is replaced by the continuous variable k. If we first consider the second-order perturbation correction for the ground state of the heavy-hole exciton we find for the exciton associated with the transition from heavy-hole level J to electron level L

$$\Delta E(J,L)=\sum_{i=1}^{4}\left[\sum_{j,n,l,m}\frac{|\langle i,j,l,n,m\,|\,H_2\,|\,1,J,L,0,0\rangle|^2}{E_{1JL00}-E_{ijlnm}}+\sum_{j,l,m}\int dk\,\frac{|\langle i,j,l,k,m\,|\,H_2\,|\,1,J,L,0,0\rangle|^2}{E_{1JL00}-E_{ijlkm}}\right]. \tag{A2}$$

It is easily verified from Eq. (13) that the sum over i gives coupling with light-hole states ($i=2,3$). The sum over l gives a factor δ_{lL} since the electron wave functions in the z direction are orthonormal. We thus find

$$\begin{aligned}\Delta E(J)&=\sum_{j,n,m}\left[\frac{|\langle j,n,m\,|\,B^*\,|\,J,0,0\rangle|^2}{E_{J00}-E_{jnm}}+\frac{|\langle j,n,m\,|\,C^*\,|\,J,0,0\rangle|^2}{E_{J00}-E_{jnm}}\right]\\&\quad+\sum_{j,m}\int dk\left[\frac{|\langle j,k,m\,|\,B^*\,|\,J,0,0\rangle|^2}{E_{J00}-E_{jkm}}+\frac{|\langle j,k,m\,|\,C^*\,|\,J,0,0\rangle|^2}{E_{J00}-E_{jkm}}\right]\\&=\sum_{j,n,m}\left[\frac{|I_j^J|^2\,|J_{nm}^{00}|^2}{E_{J00}-E_{jnm}}+\frac{|K_j^J|^2\,|L_{nm}^{00}|^2}{E_{J00}-E_{jnm}}\right]+\sum_{j,m}\int dk\left[\frac{|I_j^J|^2\,|J_{km}^{00}|^2}{E_{J00}-E_{jkm}}+\frac{|K_j^J|^2\,|L_{km}^{00}|^2}{E_{J00}-E_{jkm}}\right],\end{aligned} \tag{A3}$$

where we have defined

$$I_j^J=\left\langle j\left|\frac{\partial}{\partial z}\right|J\right\rangle, \tag{A4a}$$

$$J_{nm}^{00}=\sqrt{3}\gamma_3\left\langle n,m\left|\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right|0,0\right\rangle, \tag{A4b}$$

$$K_j^J=\langle j\,|\,J\rangle\ , \tag{A4c}$$

and

$$L_{nm}^{00}=\frac{\sqrt{3}}{2}\left\langle n,m\left|\gamma_2\left[\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}\right]+2i\gamma_3\frac{\partial^2}{\partial x\,\partial y}\right|0,0\right\rangle. \tag{A4d}$$

(We have here set $m_0=\hbar=1$.) The bound quantum-well eigenfunctions of H_0^h (and H_0^e) can be divided into even-parity solutions and odd-parity solutions. We use the common boundary conditions with continuity of the envelope function $\psi(z)$ and $(1/m)d\psi/dz$.[44] This leads to the transcendental equation

$$\tan(qb)=\frac{m_1 s}{m_2 q} \tag{A5a}$$

for even-parity states and

$$\cot(qb)=-\frac{m_1 s}{m_2 q} \tag{A5b}$$

for odd-parity states, where

$$\hbar q=\sqrt{2m_1 E} \tag{A6a}$$

and

$$\hbar s=\sqrt{2m_2(V-E)}\ . \tag{A6b}$$

V is the height of the potential barrier, m_1 is the effective mass in GaAs for the electron (m_e), for the heavy hole [$m_h=(\gamma_1-2\gamma_2)^{-1}$], or for the light hole [$m_l=(\gamma_1+2\gamma_2)^{-1}$], and m_2 is the corresponding quantity in $Al_xGa_{1-x}As$. The energy solutions E_j are obtained by solving the Eqs. (A5) numerically and insertion into Eqs. (A6) gives the corresponding q_j and s_j. We find

$$I_j^J=-A_J^t A_j^{-t}\left[\frac{tq_J\sin[(q_J-q_j)b]}{q_J-q_j}-\frac{q_J\sin[q_J+q_j)b]}{q_J+q_j}+\frac{s_J\{\sin[(q_J+q_j)b]-t\sin[(q_J-q_j)b]\}}{s_J+s_j}\right], \tag{A7}$$

$$K_j^J=A_J^t A_j^t\left[\frac{\sin[(q_J-q_j)b]}{q_J-q_j}+\frac{t\sin[(q_J+q_j)b]}{q_J+q_j}+\frac{\cos[(q_J-q_j)b]+t\cos[(q_J+q_j)b]}{s_J+s_j}\right], \tag{A8}$$

where the A^t are normalization constants in the quantum-well region given by

$$A^t=\left[b+\frac{t\sin(2qb)}{2q}+\frac{1+t\cos(2qb)}{2s}\right]^{-1/2}. \quad \text{(A9)}$$

Here $t=+1$ should be chosen if the state J has even parity, and $t=-1$ if it has odd parity. Note that expression (A8) is different from δ_{jJ} because q_J belongs to the heavy-hole function while the q_j belong to light-hole functions. It is clear from parity considerations that $I_j^J=0$ if j and J have the same parity while $K_j^J=0$ if they have opposite parities.

For the continuum quantum-well states ($E>V$) we use the additional boundary conditions $\psi\to 0$ as $z=\pm L$, where $L\gg b$. In a similar way we find that the energies are obtained from

$$\tan(qb)=\frac{m_1 p}{m_2 q}\cot[p(L-b)] \quad \text{(A10a)}$$

for the even-parity states and

$$\cot(qb)=-\frac{m_1 p}{m_2 q}\cot[p(L-b)] \quad \text{(A10b)}$$

for the odd-parity states. Here

$$\hbar p=[2m_2(E-V)]^{1/2} \quad \text{(A11)}$$

and q is given by (A6a). The matrix elements between a bound state characterized by q_J and s_J and a continuum state by q_j and p_j are the same as (A7) and (A8) if we only make the replacement

$$\frac{1}{s_J+s_j}\to\frac{s_J-p_j\cot[p_j(L-b)]}{s_J^2+p_j^2} \quad \text{(A12a)}$$

and use the normalization constant

$$A^t=\left[b+\frac{t\sin(2qb)}{2q}+\frac{1+t\cos(2qb)}{2}\left[\frac{L-b}{\sin^2[p(L-b)]}-\frac{\cot[p(L-b)]}{p}\right]\right]^{-1/2} \quad \text{(A12b)}$$

for the continuum state. In the matrix elements between bound and continuum states we have omitted a term proportional to $\exp[-s_J(L-b)]$, which is negligible for the cases we consider. The boundary conditions at $\pm L$ imply that we sum over a quasicontinuum of densely spaced states instead of integrating over true continuum states. The number of states up to a cutoff energy $E_{\max}$ increases with L, but, as is seen in Eq. (A12b), the normalization constant decreases with L. The contribution to the exciton binding energy turns out to be insensitive to L if we choose the width of the outer well $2L$ of the order 1000 Å.

We next consider the bound states of $H_0^{\rm exc}$. The eigenfunctions were given by Shinada and Sugano[22] and can in our case been written

$$\psi_{nm}^{\rm exc}(\rho,\phi)=\frac{2}{a(n+\frac{1}{2})}\frac{1}{(2\,|\,m\,|\,)!}\times\left[\frac{(n+|\,m\,|\,)!}{(n-|\,m\,|\,)!(2n+1)}\right]^{1/2}\times e^{-\tilde{\rho}/2}\tilde{\rho}^{\,|\,m\,|}F(|\,m\,|-n,2|\,m\,|+1,\rho)\times\frac{1}{\sqrt{2\pi}}e^{im\phi}, \quad \text{(A13)}$$

where

$$\tilde{\rho}=\frac{2\rho}{a(n+\frac{1}{2})}, \quad \text{(A14a)}$$

$$a=\frac{\epsilon\hbar^2}{\mu\lambda e^2}, \quad \text{(A14b)}$$

and $F(b,c,z)$ is the confluent hypergeometric function.[45] For heavy-hole states $\mu^{-1}=m_e^{-1}+\gamma_1+\gamma_2$ while $\mu^{-1}=m_e^{-1}+\gamma_1-\gamma_2$ for light-hole states. λ is the parameter introduced in Eqs. (11) and (12). The energies are given by

$$E_n=-\frac{\mu\lambda^2 e^4}{2\hbar^2\epsilon^2(n+\frac{1}{2})^2},\quad n=0,1,2,\ldots. \quad \text{(A15)}$$

The absolute value of the quantum number m is $\le n$. States with $|\,m\,|=0,1,2,\ldots$ can be denoted s, p, and d states, etc.[10] When the operator $\partial/\partial x+i\partial/\partial y$ operates on the ground-state wave function it gives a factor $\exp(i\phi)$. The ϕ integral gives $2\pi\delta_{m1}$ and thus the only nonzero term in the sum over m [Eq. (A3)] comes from $m=1$. The integral over ρ gives the result

$$J_{nl}^{00}=-\gamma_3\frac{16A}{a^2}[3(2n+1)(n+1)n]^{1/2}\times\frac{[(2n+1)\beta-1]^{n-1}}{[(2n+1)\beta+1]^{n+2}}, \quad \text{(A16)}$$

where we have used the relations[46]

$$\int_0^\infty e^{-st}t^{c-1}F(b,d,kt)dt=\Gamma(c)s^{-c}F(b,c,d,k/s) \quad \text{(A17)}$$

and

$$F(b,c,c,z)=(1-z)^{-b}. \quad \text{(A18)}$$

Here $F(b,c,d,z)$ is the hypergeometric function and $\beta=A/a$, where a is the effective Bohr radius for the heavy hole [see Eq. (A14b)] and A is that for the light hole.

The most laborious part of the calculation is the evaluation of the matrix elements L_{nm}^{00}. The operator C^* is first rewritten

$$\frac{\sqrt{3}}{2}[\gamma_2(k_x^2-k_y^2)+2i\gamma_3 k_x k_y]=\frac{\sqrt{3}}{2}(\tilde{\gamma}k_+^2-\mu k_-^2), \quad \text{(A19)}$$

where we have introduced

$$\tilde{\gamma}=(\gamma_3+\gamma_2)/2 , \tag{A20a}$$

$$\mu=(\gamma_3-\gamma_2)/2 , \tag{A20b}$$

and

$$k_{\pm}=k_x\pm ik_y . \tag{A20c}$$

When $(\partial/\partial x\pm i\partial/\partial y)^2$ operates on the ground state we obtain a factor $\exp(\pm 2i\phi)$. Thus the only contribution from the sum over m comes from $m=\pm 2$ and since the radial wave function only depends on $|m|$ we can write

$$\begin{aligned}\sum_m |L_{nm}^{00}|^2 &= \left|\left\langle n,2\left|\frac{\sqrt{3}}{2}\tilde{\gamma}k_+^2\right|0,0\right\rangle\right|^2 \\ &\quad+\left|\left\langle n,-2\left|-\frac{\sqrt{3}}{2}\mu k_-^2\right|0,0\right\rangle\right|^2 \\ &= \tfrac{3}{4}(\tilde{\gamma}^2+\mu^2)|l_n|^2=\tfrac{3}{8}(\gamma_2^2+\gamma_3^2)|l_n|^2 ,\end{aligned} \tag{A21}$$

where

$$l_n=\langle n,2|k_+^2|0,0\rangle=\langle n,-2|k_-^2|0,0\rangle . \tag{A22a}$$

We similarly define

$$l_k=\langle k,2|k_+^2|0,0\rangle . \tag{A22b}$$

Using Eq. (A17) we obtain

$$\begin{aligned}l_n=&\frac{16}{3a^2[(2n+1)\beta+1]^3}\left[\frac{(n+2)!}{(n-2)!(2n+1)}\right]^{1/2} \\ &\times\left[\frac{3\beta(2n+1)}{(2n+1)\beta+1}F\left[2-n,4,5,\frac{2}{(2n+1)\beta+1}\right]\right. \\ &\left.+F\left[2-n,3,5,\frac{2}{(2n+1)\beta+1}\right]\right] .\end{aligned} \tag{A23}$$

The hypergeometric functions are evaluated below. We first turn to the continuum states, which can be written[22]

$$\psi_{km}^{\rm exc}(\rho,\phi)=\frac{1}{(2|m|)!}\left[\frac{2k\prod_{j=1}^{|m|}[(j-\frac{1}{2})^2+\alpha^2]}{1+e^{-2\pi\alpha}}\right]^{1/2}(2k\rho)^{|m|}e^{-ik\rho}F(|m|+\tfrac{1}{2}+i\alpha,2|m|+1,2ik\rho)\frac{1}{\sqrt{2\pi}}e^{im\phi} , \tag{A24}$$

where

$$\alpha=(kA)^{-1} \tag{A25a}$$

and

$$\hbar k=\left[\frac{2E}{(1/m_e)+\gamma_1-\gamma_2}\right]^{1/2} . \tag{A25b}$$

For $m=0$ the product in Eq. (A24) is replaced by one. In a way similar to the derivation for the bound states we find

$$\begin{aligned}J_{kl}^{00}=&-\gamma_3\frac{16ka}{(4+k^2a^2)^{3/2}}\left[\frac{6k(\alpha^2+\frac{1}{4})}{1+e^{-2\pi\alpha}}\right]^{1/2} \\ &\times\exp\left[-2\alpha\tan^{-1}\left[\frac{ka}{2}\right]\right]\end{aligned} \tag{A26}$$

and

$$\begin{aligned}l_k=&\frac{8k^2a}{3(2+ika)^3}\left[\frac{2k(\alpha^2+\frac{1}{4})(\alpha^2+\frac{9}{4})}{1+e^{-2\pi\alpha}}\right]^{1/2} \\ &\times\left[\frac{6}{2+ika}F\left[5/2+i\alpha,4,5,\frac{2ika}{2+ika}\right]\right. \\ &\left.+F\left[5/2+i\alpha,3,5,\frac{2ika}{2+ika}\right]\right] .\end{aligned} \tag{A27}$$

In both Eqs. (A23) and (A27) the combination of hypergeometric functions is of the form

$$G(y,z)=3(1-z/2)F(y,4,5,z)+F(y,3,5,z) . \tag{A28}$$

Repeated use of the relation[46]

$$\begin{aligned}&(\alpha-\beta)zF(\alpha,\beta,\gamma+1,z) \\ &\quad=\gamma F(\alpha-1,\beta,\gamma,z)-\gamma F(\alpha,\beta-1,\gamma,z)\end{aligned} \tag{A29}$$

and Eq. (A18) gives

$$\begin{aligned}G(y,z)=-12&\left[\frac{2y-5}{z^3}+\left[\frac{(y-3)(y-2)(y-1)}{2}-\frac{(2y-5)(y-2)(y-1)}{2z}\right.\right. \\ &\left.\left.+\frac{(2y-5)(y-1)}{z^2}-\frac{2y-5}{z^3}\right](1-z)^{1-y}\right]\Big/[(y-4)(y-3)(y-2)(y-1)] .\end{aligned} \tag{A30}$$

We finally obtain

$$l_n=\frac{8}{a^2}\left[\frac{(n-2)!}{(n+2)!(2n+1)}\right]^{1/2}\left[2n+1-\{(2n+1)^4(\beta+1)\beta^2+(2n^2+2n-1)[(2n+1)^2\beta+1]\}\frac{[(2n+1)\beta-1]^{n-1}}{[(2n+1)\beta+1]^{n+2}}\right] \tag{A31}$$

for the bound states while the result for the continuum states becomes

$$l_k=\frac{8}{k^2a^3}\left[\frac{2k}{(\alpha^2+1/4)(\alpha^2+9/4)(1+e^{-2\pi\alpha})}\right]^{1/2} \times\left[\beta^{-1}-[4\beta^{-3}-(k^2a^2-8)\beta^{-2}+(3k^2a^2+8)\beta^{-1}-3k^4a^4/4]\frac{\exp\left[-2\alpha\tan^{-1}\left[\frac{ka}{2}\right]\right]}{(4+k^2a^2)^{3/2}}\right]. \tag{A32}$$

In the sum over n the first few terms clearly dominate and we have found it sufficient to sum over ten states. The integral over k is performed numerically with the use of a 96-point Gaussian integration routine.

The perturbation of the light-hole states can be obtained from the results above if only the effective Bohr radii a and A are suitably redefined. This amounts to replacing γ_2 by $-\gamma_2$ in the final results.

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