Exciton in a quantum-well structure for arbitrary magnetic field strengths

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The magnetic-field-strength and quantum-well-width dependence of the ground-state energies of a magnetoexciton in a GaAs/$Ga_{1-x}Al_xAs$ quantum-well structure are studied for arbitrary magnetic field strengths. The results show that the energy of the magnetoexciton will increase with increasing quantum-well width and magnetic field strength. We also found that the magnetoexciton in the $l_{e,h}=1$ state is more stable than in the $l_{e,h}=2$ state.

The problem of a hydrogenlike impurity and exciton in bulk semiconductors in a constant magnetic field of arbitrary strength has been the subject of numerous experimental and theoretical investigations. With recent technological progress in materials growth, special attention has been focused on systems with reduced dimensions,[1-7] such as superlattices and quantum-well structures. The properties of excitons in these systems in a constant magnetic field have aroused great interest, both theoretically[4,5] and experimentally.[6,7]

The coexistence of the excitonic Coulomb interaction and the magnetic-field-related terms in the Hamiltonian of a magnetoexciton system is difficult to treat theoretically because these two terms could be comparable in magnitude. Most theoretical works study only properties of magnetoexcitons in two magnetic field limits. Using the two-point Padé approximation method, MacDonald and Ritchie[8] have studied the hydrogen energy levels in a two dimensional (2D) system for arbitrary magnetic field strengths. Few works in the literature study the magnetoexciton for magnetic fields of arbitrary strengths. Furthermore, most works treat the quantum-well structure as a 2D system, while in reality it is a quasi-two-dimensional (Q2D) system.

Among quantum wells and superlattices, the GaAs/$Ga_{1-x}Al_xAs$ system appears to be the simplest and most interesting. Now, we consider a quantum well of polar crystal with width $2d$; a polar crystal 1 occupies the space for $|z|\le d$, and when $|z|\ge d$, the space is filled with crystal 2. An exciton moves inside crystal 1. Assuming that the valence-subband structure can be reduced to a single transverse effective mass, apply a uniform magnetic field $\mathbf{B}$ along the z direction and describe it according to the symmetric gauge. Under the isotropic effective-mass approximation, the Hamiltonian of the system may be written as

$$
\begin{aligned}
H &= H_e + H_h + V_{e\text{-}h}(r) \,, \\
H_e &= \frac{1}{2m_{be}}\left[\mathbf{p}_{e_\parallel} + \frac{e}{2c}\mathbf{B}\times\boldsymbol{\rho}_e\right]^2 + \frac{\mathbf{p}_{ez}^2}{2m_{be}} + V_e(z_e) \,, \\
H_e &= \frac{1}{2m_{bh}}\left[\mathbf{p}_{h_\parallel} - \frac{e}{2c}\mathbf{B}\times\boldsymbol{\rho}_h\right]^2 + \frac{\mathbf{p}_{hz}^2}{2m_{bh}} + V_h(z_h) \,, \\
V_{e\text{-}h}(r) &= -\frac{e^2}{\epsilon_1|r_e-r_h|} \,,
\end{aligned}
\tag{1}
$$

where $\mathbf{p}_e,\mathbf{p}_h$, and $\boldsymbol{\rho}_e,\boldsymbol{\rho}_h$ are the momenta and coordinates of the electron and hole, respectively, in the xy plane. ϵ_1 is the dielectric constant of crystal 1.

First, let us rewrite the Hamiltonian in the center-of-mass system, then perform a unitary transformation with

$$
U=\exp\left[\frac{i}{\hbar}\left[\mathbf{K}+\frac{e}{2c}\mathbf{B}\times\mathbf{R}\cdot\boldsymbol{\rho}\right]\right] \,, \tag{2}
$$

where $\mathbf{R}$ and $\boldsymbol{\rho}$ are the center-of-mass and relative coordinates, respectively, and $\mathbf{K}$ is the total momentum. As shown in Ref. 4, the states of interest in optical transition are only those in which $\mathbf{K}=\mathbf{0}$. After some algebraic manipulations, we find the transformed Hamiltonian as

$$
\begin{aligned}
H &= H_\parallel + H_\perp + H_I \,, \\
H_\parallel &= \frac{1}{2\mu}\left[\mathbf{p}_\rho + \frac{e}{2c}\mathbf{B}\times\boldsymbol{\rho}\right]^2 - \frac{e}{cm_{bh}}\mathbf{B}\times\boldsymbol{\rho}_\rho\cdot\mathbf{p} - \frac{\lambda e^2}{\epsilon_1\rho} \,, \\
H_\perp &= \frac{\mathbf{p}_{ez}^2}{2m_{be}} + \frac{\mathbf{p}_{hz}^2}{2m_{bh}} + V_e(z_e) + V_h(z_h) \,, \\
H_I &= \frac{\lambda e^2}{\epsilon_1\rho} - \frac{e^2}{\epsilon_1[\rho^2+(z_e-z_h)^2]^{1/2}} \,,
\end{aligned}
\tag{3}
$$

where $\mu = m_{be}m_{bh}/(m_{be}+m_{bh})$ is the reduced mass of the exciton and $\mathbf{p}_\rho$ is the relative momentum of the exciton. We have introduced the plane Coulomb potential[9] with the parameter λ and, as will be seen later, λ can be determined by perturbation theory.

For a narrow quantum well, the motion of the exciton along the z axis is almost in a certain state; therefore, we can employ the quasiadiabatic approximation[10] to find the effective Hamiltonian of the system. We first seek the expected value of $H_\parallel$, which depends on the parameter z. Then we add the expected value, as an adiabatic potential, to $H_\perp$ in order to obtain the effective Hamiltonian.

In the Hamiltonian representation, $H_\parallel$ is the Hamiltonian of the "two-dimensional" exciton in the magnetic field with the λ-dependent excitonic Coulomb interaction potential, and $H_\perp$ is the Hamiltonian of the electron (hole) moving along the z direction, which is not affected by the magnetic field. $\gamma = \hbar\omega_c/2\mathcal{R}^*$ is used to describe the strength of the magnetic field relative to the Coulomb interaction, where $\mathcal{R}^* = \mu e^4/2\hbar^2\epsilon_1^2$ is the effective rydberg and $\omega_c = eB_M/\mu c$ is the cyclotron-resonance frequency.

We first treat $H_\parallel$ in the strong magnetic field limit, that is, $\gamma \gg 1$; the λ-related two-dimensional Coulomb potential can be treated as a perturbation. The unperturbed Hamiltonian of $H_\parallel$ is just the Hamiltonian of a "free electron" under the influence of the perpendicular magnetic field.

The eigenvalues of $H_\parallel$ can be written as[8,11]

$$E_{N,M}(z) = E_{N,M}^{(0)} + E_{N,M}^{(1)} + E_{N,M}^{(2)} + E_{N,M}^{(3)} + E_{N,M}^{(4)} + \cdots , \tag{4}$$

where

$$E_{N,M}^{(0)} = \hbar\omega_c \left[N + \frac{1}{2} \right] - (N-M)\frac{\hbar e B}{m_{bh} c} , \quad N = 0,1,2,\ldots, \quad M = 0,1,2,\ldots, \tag{5}$$

and $E_{N,M}^{(i)}$ $(i = 1,2,3,\ldots)$ are the correction energies given in Refs. 8 and 11.

Then we discuss the behavior of the magnetoexciton in the weak magnetic field limit, i.e., $\gamma \ll 1$; the second term in $H_\parallel$ can be treated as a perturbation. The energy eigenvalues up to the third order in γ and eigenfunction are[8]

$$\begin{aligned} E_{n,m} &= \frac{e^2\lambda^2}{2\epsilon_1 a_0^*(n-1/2)^2} + m\frac{eB_M\hbar}{2\mu_- c} + \frac{e^2B_M^2}{8c^2\mu^2}\langle\rho^2\rangle_{n,m} + O(\gamma^4) , \\ \phi_{n,m}(\rho,\lambda) &= \frac{1}{\sqrt{2\pi}} e^{im\varphi} R_{n,m}\left[\frac{2\rho\lambda}{(n-1/2)a_0^*} \right] , \end{aligned} \tag{6}$$

where $a_0^* = \epsilon_1\hbar/\mu e^2$ are the effective Bohr radii,

$$\mu_- = m_{bh}m_{be}/(m_{bh}-m_{be}) ,$$

and

$$\langle\rho^2\rangle_{n,m} = \int_0^{2\pi} d\varphi \int_0^\infty \rho^3\phi_{n,m}^2(\rho,\lambda)d\rho . \tag{7}$$

In the intermediate magnetic field regime, i.e., $\gamma \to 1$, we use the two-point Padé approximation suggested by MacDonald and Ritchie[8] to interpolate between the weak and strong magnetic field extremes. We denote the kth eigenvalue, with azimuthal quantum number m, as $\Pi_{k,m}$ $(k = 1,2,3,\ldots)$. The energy levels for the two field extremes can be written as

$$\Pi_{k,m}(v) = \begin{cases} \sum_{i=0}^{7} \eta_{k,m}^{(i)} v^i + O(v^8) & \text{as } v \to 0 \\ v^2 \sum_{i=0}^{4} \xi_{k,m}^{(i)} v^{-i} + O(v^{-5}) & \text{as } v \to \infty , \end{cases} \tag{8}$$

where $v = \sqrt{\gamma}$, and η and ξ are the numerical coefficients. The $[L/M]$ two-point Padé approximate $\Pi_{kmn}^{(s,t)}(v)$ is

$$\Pi_{k,m}^{(s,t)}(v) = \frac{P_{k,m}^L(v)}{Q_{k,m}^M(v)} = \frac{p_0 + p_1 v + p_2 v^2 + \cdots + p_L v^L}{1 + q_1 v + q_2 v^2 + \cdots + q_M v^M} \tag{9}$$

and can be formed by requiring

$$\Pi_{k,m}(v) - \Pi_{k,m}^{(s,t)}(v) = O(v^{s+1}, v^{-(t+1)}) , \tag{10}$$

that is, the left-hand side reduces to $O(v^{s+1})$ as $v \to 0$ and to $O(v^{-(t+1)})$ as $v \to \infty$, respectively. You can see the details of the two-point Padé approximations in Ref. 8.

For a narrow quantum well, we assume that

$$V_e(z_e), V_h(z_h) = \begin{cases} 0, & |z_e|,|z_h| \le d \\ \infty, & |z_e|,|z_h| \ge d , \end{cases} \tag{11}$$

i.e., we assume the electron (hole) is moving in a one-dimensional infinite-depth square-potential well, so that the eigenfunctions and eigenenergies of $H_\perp$ are

$$\begin{aligned} |\phi_{l_e}(z_e)\rangle|\phi_{l_h}(z_h)\rangle &= \begin{cases} \frac{1}{d}\sin\left[\frac{l_e\pi}{2d}(z_e+d)\right]\sin\left[\frac{l_h\pi}{2d}(z_h+d)\right], & |z_e|,|z_h| \ge d \\ 0, \quad |z_e|,|z_h| \ge d \end{cases} \\ E_{l_e l_h} &= \frac{\pi^2\hbar^2 l_e^2}{8m_{be}d^2} + \frac{\pi^2\hbar^2 l_h^2}{8m_{bh}d^2}, \quad l_e, l_h = 1,2,3,\ldots,N \end{aligned} \tag{12}$$

where $Na = 2d$, and a is the lattice constant.

According to the perturbation method,[9] for a narrow quantum well, the difference between λ/ρ and $1/[\rho^2+(z_e-z_h)^2]^{1/2}$ can be made very small by choosing an applicable value of λ; therefore, the expected value of the perturbation term H_I should be set to zero in a narrow quantum well, i.e.,

$$\overline{H}_I(\lambda)=\langle \phi_{le}(z_e)\phi_{lh}(z_h)\Psi_{N,M}(x,y)|H_I \times|\phi_{le}(z_e)\phi_{lh}(z_h)\Psi_{N,M}(x,y)\rangle=0 \ . \tag{13}$$

Thus, the relevant parameter λ can be determined, which we express as $\lambda_{\min}$.

Taking the exciton in the $GaAs/Ga_{1-x}Al_xAs$ quantum-well structure as an example, we perform the numerical evaluation. The characteristic parameters of GaAs are listed as follows: $\epsilon_1=12.83$, $m_{be}=0.0657m_0$, $m_{bh}=0.12m_0$, and $a=5.654$ Å.

The effect of the Coulomb potential is related to the width of the quantum well. Figure 1 shows the parameter $\lambda_{\min}$ as a function of the width of the quantum well N in two extreme magnetic field limits. We can see that $\lambda_{\min}$ decreases with increasing quantum-well width; that is to say, the effect of the Coulomb potential is weakened with increasing width of the quantum well. The narrower the quantum well, the stronger the effect of the exciton Coulomb potential, and we can also see that $\lambda_{\min}$ in the $l_e,l_h=1$ state is larger than that in the $l_e,l_h=2$ state.

In the weak magnetic field limit, $\lambda_{\min}$ hardly depends on the magnetic field strength, but it will decrease with

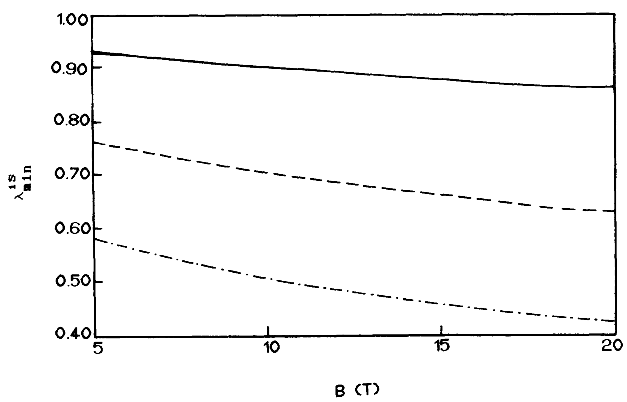

FIG. 2. The dependence of the parameters $\lambda_{\min}$ of the 1s state on magnetic field strength in the high-field limit for $N=10$ (solid line), $N=40$ (dashed line) and $N=100$ (dot-dashed line); $l_{e,h}=1$.

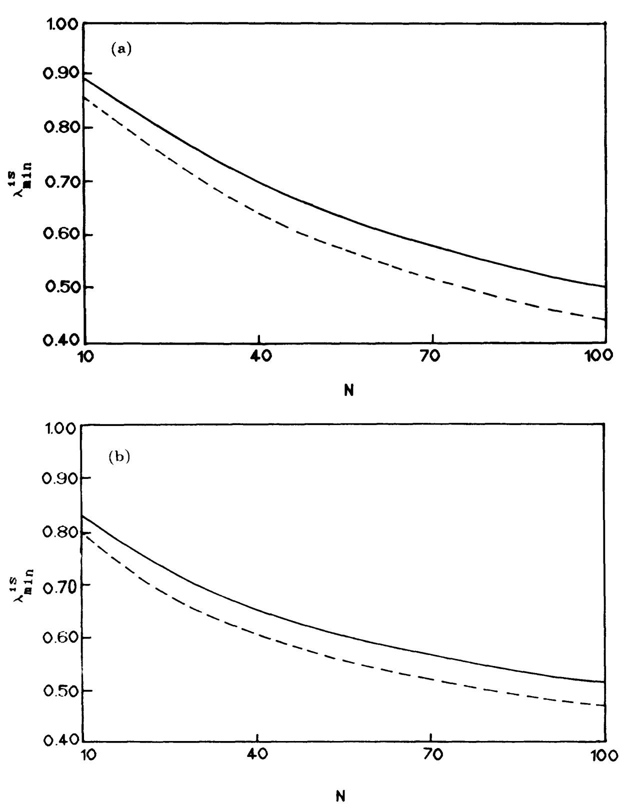

FIG. 1. The dependence of the parameters $\lambda_{\min}$ of the 1s state on quantum-well width N ($Na=2d$) in (a) the low-magnetic-field limit; (b) the high-magnetic-field limit for $l_{e,h}=1$ (solid line) and $l_{e,h}=2$ (dashed line).

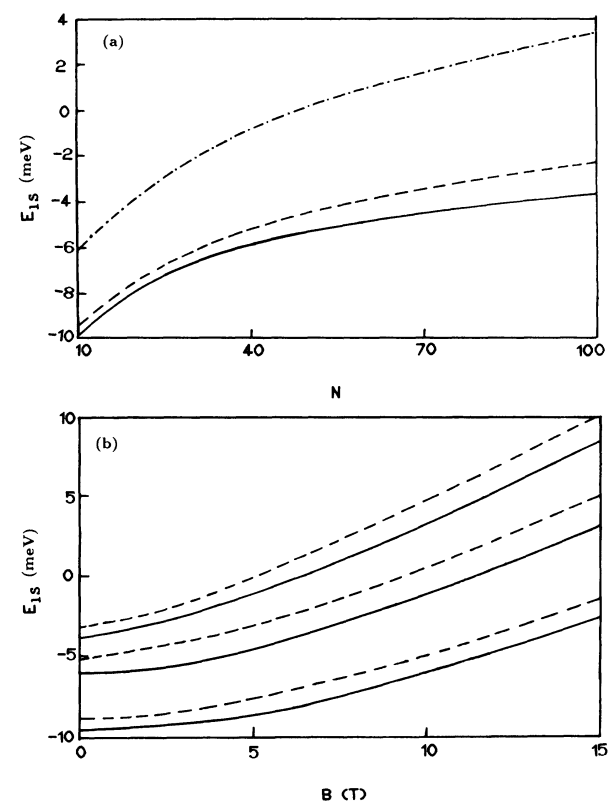

FIG. 3. The dependence of the exciton energy (excluding the contribution from the z direction) in the 1s state on (a) quantum-well width N for different magnetic field strengths $B=0$ T (solid line), $B=3$ T (dashed line), and $B=10$ T (dot-dashed line); (b) magnetic field strength B for quantum-well widths $N=10$, 40, and 100 (from bottom to top) for $l_{e,h}=1$ (solid line) and $l_{e,h}=2$ (dashed line).

increasing magnetic field strength in the strong magnetic-field limit. Figure 2 shows the magnetic-field-strength dependence of $\lambda_{\min}$ for quantum-well width $N=10$, 40, and 100. We can see that the narrower the quantum-well width, the less the change of $\lambda_{\min}$ with the magnetic field strength. So, for narrow quantum-well structures, the effect of the magnetic field on the exciton Coulomb potential is very small.

Now we will give our numerical results of the exciton energies for arbitrary magnetic field strength. For the first several ground states, we can use the [7/4] ($s=7$, $t=4$) two-point Padé approximation to evaluate the eigenenergies of the exciton.[8] The coefficients of $Q_M(v)$ are determined from the following linear equations:

$$\begin{bmatrix} -\eta_6 & -\eta_5 & -\eta_4 & -\eta_3 & \xi_0-\eta_2 \\ -\eta_5 & -\eta_4 & -\eta_3 & \xi_0-\eta_2 & \xi_1-\eta_1 \\ -\eta_4 & -\eta_3 & \xi_0-\eta_2 & \xi_1-\eta_1 & \xi_2-\eta_0 \\ -\eta_3 & \xi_0-\eta_5 & \xi_1-\eta_4 & \xi_2-\eta_3 & \xi_3 \\ \xi_0-\eta_2 & \xi_1-\eta_5 & \xi_2-\eta_4 & \xi_3-\eta_3 & \xi_4 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \end{bmatrix} = \begin{bmatrix} \eta_7 \\ \eta_6 \\ \eta_5 \\ \eta_4 \\ \eta_3 \end{bmatrix} \tag{14}$$

and the coefficients of $P_L(v)$ are determined directly from $Q_M(v)$ as

$$p_k=\sum_{i=0}^{k}\eta_{k-i}q_l,\quad k=0,1,2,\ldots, \tag{15}$$

where η and ξ are the coefficients, which are decided by Eqs. (4), (6), and (8).

The behavior of a magnetoexciton depends primarily on $H_{\parallel}$, because $H_{\perp}$ is unaffected by the magnetic field. Figure 3 shows the exciton energies in the ground state as a function of magnetic field strength and quantum-well width. We can see from Figure 3 that the energies of the magnetoexciton in quantum-well structures are an increasing function of the magnetic field strength and the quantum-well width. The narrower the quantum well, the smaller the energies of the magnetoexciton, that is to say, the exciton state is more stable for the narrow quantum well. Furthermore, the larger the magnetic field strength, the larger the energies of the magnetoexciton, i.e., the magnetic field will weaken the stability of the magnetoexciton. We can also see that the energies of the magnetoexciton in the $l_{e,h}=2$ state are larger than those in the $l_{e,h}=1$ state; that is to say, the magnetoexciton in the $l_{e,h}=1$ state is more stable than in the $l_{e,h}=2$ state.

Finally, for the Q2D quantum-well structure the behavior of the magnetoexciton is strongly correlated with the width of the quantum well and the strength of the magnetic field, and so we do not treat it as a pure 2D problem. We plan to study further the properties of the magnetoexciton-phonon system in Q2D systems.

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