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Magnetoexciton binding energies in a quantum wire

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Abstract

Binding energies of the 1s and $2p_{\pm}$ states of a heavy-hole Wannier exciton are calculated in an infinite-length cylindrical GaAs–$Ga_{1-x}Al_xAs$ quantum wire, under the action of a magnetic field applied in the axial direction of the wire. The calculations are made using a variational method and the effective-mass approximation for a finite confinement potential. Also, the transition energies $1s \rightarrow 2p_{\pm}$ are calculated for the same system. We have found that $2p_{\pm}$ states are not bounded for some values of the radius of the wire and of the applied magnetic field. We show how the applied magnetic field splits the degeneracy of the states with $n = 2$. Our results are compared with those obtained by other authors and with recent experimental results.

1. Introduction

Correlated electron–hole pairs form excitons in semiconductor heterostructures. The electron–hole interaction in semiconductor nano-structures is increased for the geometrical confinement, which increases the overlap of the electron and hole wave functions. The size of the nano-structure and the height of the confinement potential as well as electric and magnetic fields determine this overlap. For example the binding energy of the exciton increases when the dimensionality of the system is diminished. The optical properties of direct gap semiconductors reveal the existence of excitons as well as the different transitions between their excited states. Lerner and Lozovik [1] investigated, for the first time, the properties of excitons in low-dimensionality systems in the presence of a high magnetic field in 1978, a matter that has been the reason for numerous investigations from then on. The structure of the excitons in wells and wires has been revealed by means of extensive studies of interband spectroscopy of one and two photons [2], studies of the photoluminescence excitation spectra (PLE) of resolved polarization [3], magnetophotoluminescence [4] and photoluminescence (PL) [5]. Černe *et al* [6] have investigated the terahertz dynamics of magnetoexcitons in GaAs/GaAlAs undoped multiple quantum wells (MQWs) under magnetic fields applied perpendicular to the well interfaces, and observed resonant far-infrared (FIR) absorption by the confined magnetoexcitons. They have assigned to the $1s \rightarrow 2p_+$ intraexcitonic transition of the heavy-hole exciton the dominant resonance in GaAs/$Ga_{0.7}Al_{0.3}As$ MQWs. The absorption feature was found to persist even when the FIR electric field is comparable to the electric field that binds the exciton. Salib *et al* [7] made a detailed optically detected resonance (ODR) experimental

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study of internal transitions of confined magnetoexcitons in two GaAs/$Ga_{0.7}As_{0.3}$Al MQW structures (125 Å well/150 Å barrier, and 80 Å well/150 Å barrier), with several resonances assigned to $1s \rightarrow 2p_+$, $1s \rightarrow 3p_+$ and $1s \rightarrow 4p_+$ internal excitonic transitions. Duque *et al* [8] have studied the internal transitions of confined magnetoexcitons in GaAs–(Ga, Al)As quantum wells, finding that it is necessary to include the hole subband mixing in order to have a good agreement with the experimental work reported by Černe *et al* [6].

Gang *et al* [9] calculated the ground-state binding energy of an exciton confined in a cylindrical quantum wire in the presence of a magnetic field applied in the axial direction, finding that the binding energy increases with the applied magnetic field. In [5], Someya *et al* reported the photoluminescence spectra of a series of T-shaped GaAs quantum wires (QWWs), by means of which they calculated the ground-state binding energy of a one-dimensional exciton, finding that it is enhanced upon increasing the one-dimensional confinement.

Glutsch and Chemla [10] have calculated the optical absorption of QWWs for a large variety of wire radius. Optical absorption of wide quantum wires has been studied by Forshaw and Whittaker [11] to investigate the exciton binding energy as well as the oscillator strength as a function of confinement. Graf *et al* [12] calculated binding energies and linear-optical properties of quasi-one-dimensional excitons in a quantum wire in strong magnetic fields, using a one-dimensional parabolic potential, finding that magnetoexciton states are bound and possess a hydrogenic spectrum with an infinite number of bound states and a continuum of scattering states at higher energies. Xia and Cheah [14] calculated the binding energy of the ground-state exciton in T-shaped quantum wires, demonstrating that no one-dimensional hole confinement is necessary for the formation of a one-dimensional exciton. Xia and Cheah [14] studied exciton states in isolated and semi-isolated QWW, finding that the image charges have a large effect on the effective Coulomb potential in wires. In isolated wires they found that the exciton binding energy is about ten times as large as in the quantum well. Bayer *et al* [15] made systematic studies of the effect of confinement and reduced dimensionality on excitons in GaAs–(In, Al)As QWWs and in QDs. Within the variational approach they calculated the exciton binding energies and the diamagnetic shift, finding very good agreement with experiment. Siarkos and Runge [16] made numerical multiband calculations of quantum-wire excitons including valence band $\boldsymbol{k} \cdot \boldsymbol{p}$ coupling. These are based on a real-space formulation.

In this work, using the effective-mass approximation within the variational approach, we calculate the binding energy of the 1s and the $2p_\pm$ excited states, as well as the transition energies associated with the 1s and $2p_\pm$ states of an exciton located in a cylindrical GaAs–$Ga_{1-x}Al_xAs$ QWW under the action of a magnetic field applied in the axial direction. The quantum wire length is large enough to consider that the motion of the carriers is free in the axial direction. In section 2 we present the theory followed for this calculation. Our results and discussion are presented in section 3 and conclusions are summarized in section 4.

2. Theory

We consider a heavy-hole Wannier exciton confined in a cylindrical quantum wire of GaAs/$Ga_{0.7}Al_{0.3}As$ under the action of a magnetic field, applied in the axial direction of the wire. Using the effective-mass approximation and a variational scheme, the Hamiltonian of a correlated electron–hole pair is written as

$$\boldsymbol{H} = \frac{1}{2m_e}\left[\boldsymbol{P}_e + \frac{e}{c}\boldsymbol{A}_e\right]^2 + \frac{1}{2m_h}\left[\boldsymbol{P}_h - \frac{e}{c}\boldsymbol{A}_h\right]^2 - \frac{e^2}{\varepsilon|\boldsymbol{r}_e - \boldsymbol{r}_h|} + V_e(\rho_e) + V_h(\rho_h) \tag{1}$$

where

$$|\boldsymbol{r}_e - \boldsymbol{r}_h| = \sqrt{\rho_e^2 + \rho_h^2 - 2\rho_e\rho_h\cos(\varphi_e - \varphi_h) + z^2} \tag{2}$$

is the separation of the electron–hole pair, ε is the dielectric constant of GaAs, m_e and m_h are the effective masses of the electron and of the heavy hole, respectively. z is the separation, $(z_e - z_h)$, of the electron and the heavy hole in the axial direction of the wire. $\boldsymbol{A}_{e(h)}$ is the vector potential of the magnetic field that is expressed as

$$\boldsymbol{A}_{e(h)} = \frac{\boldsymbol{B} \times \boldsymbol{r}_{e(h)}}{2} \tag{3}$$

with $\boldsymbol{B} = B\underline{\boldsymbol{z}}$; the components of the vector potential in cylindrical coordinates are $A_\rho = A_z = 0$, $A_{\varphi[e(h)]} = B\rho_{e(h)}/2$, and the confinement potential of the carriers is

$$V_{e(h)}(\rho_{e(h)}) = \begin{cases} 0 & \rho_{e(h)} \leqslant R \\ V_0 & \rho_{e(h)} > R. \end{cases} \tag{4}$$

V_e, V_h are the confinement potentials of the electron and hole, respectively. In our calculations we use the values for V_e, V_h given in [17, 18] as a function of the energy gap as follows:

$$V_e = \begin{cases} 0.85\ E_g \\ 0.60\ E_g \end{cases} \qquad V_h = \begin{cases} 0.15\ E_g \\ 0.40\ E_g \end{cases} \qquad E_g = 1.155x + 0.37x^2. \tag{5}$$

As done by Gang *et al* [9], the trial wave functions are chosen as the product of a hydrogenic function and radial solutions of a carrier in the state of lower energy, in a cylindrical box under the action of a magnetic field. In this way, the wave function for any state is given by

$$\Psi(\boldsymbol{r}_e, \boldsymbol{r}_h) = \begin{cases} N \exp\left[-\dfrac{\xi_e + \xi_h}{2}\right] 1F1(a_{01_{(e)}}, 1, \xi_e) & \\ \quad \times 1F1(a_{01_{(h)}}, 1, \xi_h)\Gamma_{nlm}(r, \lambda_{nl}) & \rho_{e(h)} \leqslant R \\ N \dfrac{1F1(a_{01_{(e)}}, 1, \xi_{R_{(e)}})}{U(a'_{01_{(e)}}, 1, \xi_{R_{(e)}})} \exp\left[-\dfrac{\xi_e + \xi_h}{2}\right] & \\ \quad \times U(a'_{01_{(e)}}, 1, \xi_e) 1F1(a_{01_{(h)}}, 1, \xi_h) & \\ \quad \times \Gamma_{nlm}(r, \lambda_{nl}) & \rho_e > R \text{ and } \rho_h \leqslant R \\ N \dfrac{1F1(a_{01_{(h)}}, 1, \xi_{R_{(h)}})}{U(a'_{01_{(h)}}, 1, \xi_{R_{(h)}})} \exp\left[-\dfrac{\xi_e + \xi_h}{2}\right] & \\ \quad \times 1F1(a_{01_{(e)}}, 1, \xi_e) U(a'_{01_{(h)}}, 1, \xi_h) & \\ \quad \times \Gamma_{nlm}(r, \lambda_{nl}) & \rho_e \leqslant R \text{ and } \rho_h > R \\ N \dfrac{1F1(a_{01_{(e)}}, 1, \xi_{R_{(e)}})}{U(a'_{01_{(e)}}, 1, \xi_{R_{(e)}})} \dfrac{1F1(a_{01_{(h)}}, 1, \xi_{R_{(h)}})}{U(a'_{01_{(h)}}, 1, \xi_{R_{(h)}})} & \\ \quad \times \exp\left[-\dfrac{\xi_e + \xi_h}{2}\right] U(a'_{01_{(e)}}, 1, \xi_{R_{(e)}}) & \\ \quad \times U(a'_{(h)}, 1, \xi_{(h)})\Gamma_{nlm}(r, \lambda_{nl}) & \rho_e \text{ and } \rho_h > R \end{cases} \tag{6}$$

where $\xi_{e(h)} = (m_{e(h)}\gamma_{e(h)}/2\mu)\rho^2_{e(h)}$ and $\xi_{R_{(e)}(R_{(h)})} = m_{e(h)}\gamma_{e(h)}R^2_{e(h)}/2\mu$. μ is the reduced mass of the heavy-hole exciton and $\Gamma_{nlm}(r, \lambda_{nl})$ are hydrogenic wave functions. Equation (6) satisfies the boundary conditions $(\partial\Psi_{int}/\partial\rho_{e(h)})|_{\rho_{e(h)}=R} = (\partial\Psi_{ext}/\partial\rho_{e(h)})|_{\rho_{e(h)}=R}$, where $a_{01_{e(h)}}$ and $a'_{01_{e(h)}}$ are determined in the appendix. The effective masses of the carriers are assumed constant (with their values in GaAs) in both materials. m_h and μ can be expressed in terms of the Kohn–Luttinger band parameters γ_1 and γ_2 [17, 19] as

$$\begin{aligned} \frac{1}{m_h} &= \frac{1}{m_0}(\gamma_1 - 2\gamma_2) \\ \frac{1}{\mu} &= \frac{1}{m_e} + \frac{1}{m_0}(\gamma_1 + \gamma_2). \end{aligned} \tag{7}$$

We have assumed that the dielectric constant is the same in the two semiconductors. The hydrogenic wave functions are given by

$$\Gamma_{1s} = \exp[-\lambda_{1s}|\boldsymbol{r}_e - \boldsymbol{r}_h|]$$
$$\Gamma_{2p_\pm} = \rho_e^{|m|/2}\rho_h^{|m|/2}\exp[\mathrm{i}m(\varphi_e - \varphi_h)]\exp[-\lambda_{2p\pm}|\boldsymbol{r}_e - \boldsymbol{r}_h|]. \tag{8}$$

The binding energy $E_b(R, B)$ for the exciton is defined as the difference between the ground-state energy of the uncorrelated electron–hole system and the total energy of the correlated electron–hole pair, that is

$$E_b(R, B) = E_{0e} + E_{0h} - \langle H(R, B)\rangle. \tag{9}$$

E_{0e} and E_{0h} are the energies of the ground-state subbands for the electron and hole, respectively. These subband energies are determined solving numerically the transcendental equations for the electron and hole in each case:

$$\frac{1F1(a_{01_{e(h)}}, 2, \xi_R)}{1F1(a_{01_{e(h)}}, 1, \xi_R)} + \frac{a'_{01_{e(h)}}}{a_{01_{e(h)}}}\frac{U(a'_{01_{e(h)}} + 1, 2, \xi_R)}{U(a'_{01_{e(h)}}, 1, \xi_R)} = 0. \tag{10}$$

For computational purposes the binding energy, $E_b(R, B)$, is expressed in rydbergs ($R^* = \hbar^2/2\mu a_0^2$), where a_0 is the exciton effective Bohr radius. The values of the physical parameters for GaAs [17] used in our calculations are $m_e = 0.067m_0$, the effective mass of the electron, and $m_h = 0.135m_0$, the effective mass of the hole, where m_0 is the bearing electron mass. $\varepsilon = 12.5$, $\gamma_1 = 7.36$ and $\gamma_2 = 2.57$, $\mu = 0.0447m_0$. Following Gang *et al* [9], we have assumed an isotropic hole mass for mathematical convenience as

$$\frac{1}{m_h} = \frac{2}{3m_h(x, y)} + \frac{1}{3m_h(z)}. \tag{11}$$

3. Results and discussion

In figure 1 we present the exciton binding energy, E_b, for the 1s state as a function of the radius of the wire and for several values of the applied magnetic field. The confinement potentials are 0.85 E_g and 0.15 E_g for the electron and the heavy hole, respectively. The Al concentration is $x = 0.3$. For a given value of the magnetic field, the binding energy increases from its value in bulk (GaAs) as the radius of the wire decreases, reaching a maximum value, and then decreases to the value of the binding energy in the bulk of GaAlAs. This behaviour is due to the compressing of the excitonic wave function as the radius of the wire is diminished. For small values of the wire radius, the wave function begins to leak toward the GaAlAs material and the binding energy diminishes until it attains the characteristic value of the binding energy in the bulk of GaAlAs. For a given radius of the wire the binding energy increases with the magnetic field due to the increase in the compression of the wave function.

In figure 2 we display the binding energy for the 1s state of a heavy-hole exciton as a function of the radius of the wire and for several values of the applied magnetic field. The confinement potentials are 0.60 E_g and 0.40 E_g for the electron and the heavy hole, respectively, with the Al concentration equal to 0.3. The qualitative behaviour of the binding energy is similar to that in the previous case (figure 1). For values of the radius $R > 1\ a_0$, the binding energy in both figures has approximately the same value. The maximum of the binding energy is lower in figure 2 than in figure 1 and it is found for higher radius of the wire. Effectively, for radius of the wire $R > 1\ a_0$, the exciton feels approximately the same confinement potential, while for $R < 1\ a_0$, the exciton experiences the 0.6 E_g and 0.4 E_g electron and hole confinement potentials as if it were less confined than in the 0.85 E_g and 0.15 E_g confinement potential case.

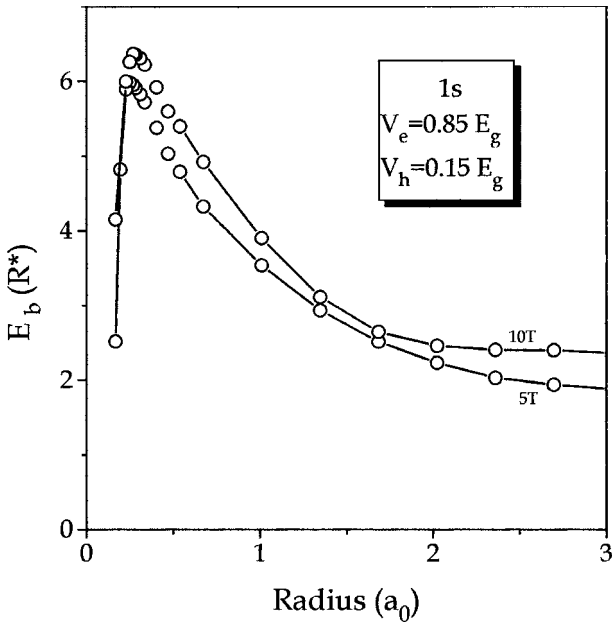

Figure 1. Binding energy, E_b, of a heavy-hole Wannier exciton in a cylindrical GaAs–(Ga, Al)As quantum-well wire as a function of the radius and for two values of the applied magnetic field. The confinement potentials for the electron and hole are 0.85 E_g and 0.15 E_g, respectively.

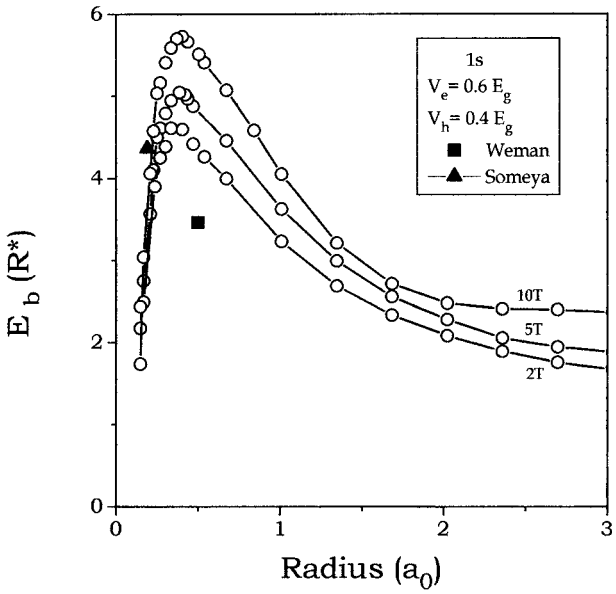

Figure 2. Binding energy, E_b, of a heavy-hole Wannier exciton in a cylindrical GaAs–(Ga, Al)As quantum-well wire as a function of the radius and for three values of the applied magnetic field. The confinement potentials for the electron and hole are 0.60 E_g and 0.40 E_g, respectively.

When the exciton is less confined, the maximum of the binding energy is found at larger radius and with a lower energy value.

Someya *et al* [5] determined in T-shaped quantum wires of GaAs/GaAlAs and of cross section 5 nm × 5 nm (that would correspond to a radius of 28 Å in a cylindrical wire) that the binding energy is 17 ± 3 meV ($4.36 \pm 0.77\ R^*$). Weman *et al* [3] reported measurements of the binding energy of excitons in coupled quantum wire arrangements directly determined from magnetoexciton excitation spectra (PLE). They found that the binding energy is 13.5 ± 0.5 meV ($3.46 \pm 0.13\ R^*$). Our results are in very good agreement with those of Someya *et al* [5] and higher than those of Weman *et al* [3]. This is because the T-shaped structure confines the excitons as efficiently as a cylindrical quantum wire, while in a superlattice the exciton confinement is weaker than in the structures mentioned above.

In figure 3 we present the binding energy of the $2p_-$ state of the exciton as a function of the radius of the wire and for three values of the magnetic field. We observe that this state is unbounded in wires with radius less than 1.5 a_0 and 1.75 a_0 for magnetic fields of 10 and 5 T, respectively. Also, there exists a crossover in the binding energy for these values of the magnetic field when the radius of the wire is close to 2.1 a_0.

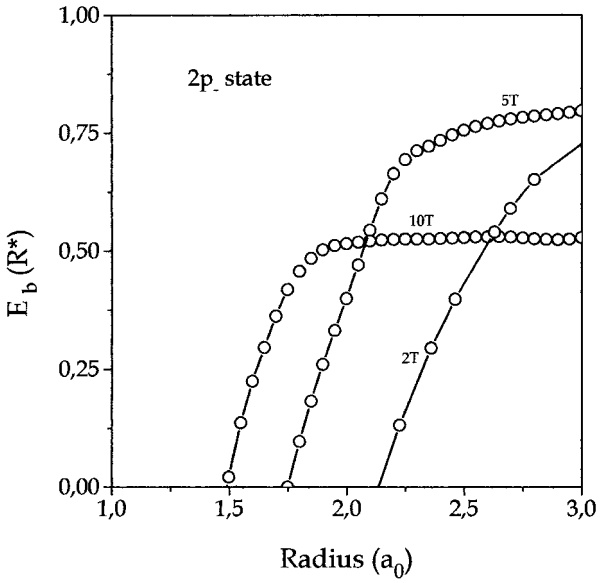

Figure 3. Binding energy of the $2p_-$ state of a heavy-hole Wannier exciton in a cylindrical GaAs–(Ga, Al)As quantum-well wire as a function of the radius and for three values of the applied magnetic field. The confinement potentials for the electron and hole are 0.60 E_g and 0.40 E_g, respectively.

The binding energy of the 1s and $2p_\pm$ excitonic states as a function of the magnetic field in a wire of radius equal to 300 Å is shown in figure 4. The binding energy of the 1s state of the exciton presents a small linear increase with the magnetic field because the excitonic wave function is not strongly confined by relatively large magnetic fields. In our calculations the excitonic effective Bohr and cyclotronic radii are approximately the same for the high magnetic fields we use in this work. The binding energy of the $2p_-$ state increases with the magnetic field and it is unbounded for magnetic fields smaller than 3 T. Also, it is seen that in a QWW of radius equal to 300 Å, the $2p_+$ state is unbounded for all the values of the magnetic field.

In figure 5 we present the energies for the transitions $1s \rightarrow 2p_-$ and $1s \rightarrow 2p_+$ as a function of the applied magnetic field. We observe that the energy for the transition $1s \rightarrow 2p_+$ is higher than that for the transition $1s \rightarrow 2p_-$ for all the values of the magnetic field. These transition energies are higher than those in quantum wells [8] and in bulk material.

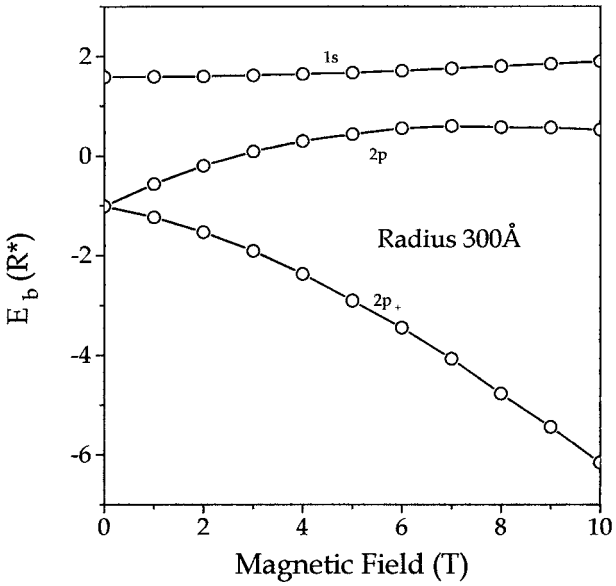

Figure 4. Binding energy, E_b, of different states of a heavy-hole Wannier exciton in a cylindrical GaAs–(Ga, Al)As quantum-well wire of radius $R = 300$ Å as a function of the magnetic field applied in the axial direction of the wire.

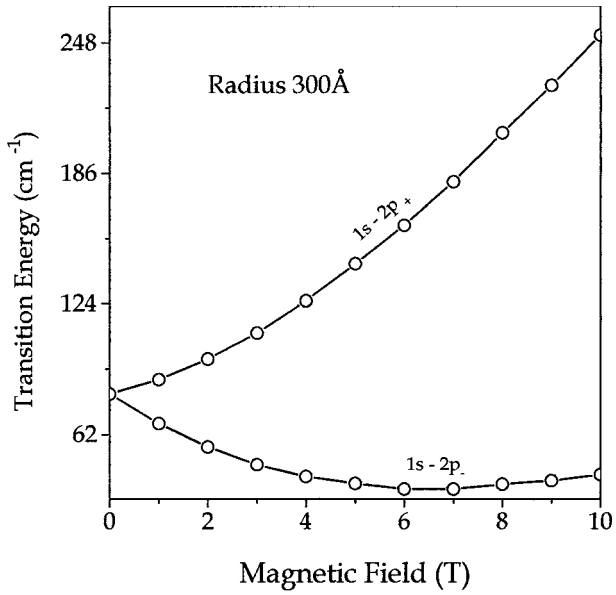

Figure 5. $1s \rightarrow 2p_-$, $1s \rightarrow 2p_+$ transition energies of a heavy-hole Wannier exciton in a cylindrical GaAs–(Ga, Al)As quantum-well wire of radius $R = 300$ Å as a function of the magnetic field applied in the axial direction of the wire.

4. Conclusions

In this work we have calculated the binding energies of the 1s and $2p_\pm$ states of a heavy-hole Wannier exciton in an infinite-length cylindrical GaAs–$Ga_{1-x}Al_xAs$ quantum wire, under the

action of a magnetic field applied in the axial direction of the wire. The calculations have been made using the effective-mass approximation within a variational scheme and for a finite confinement potential. Also, we have calculated the $1s \rightarrow 2p_{\pm}$ transition energies for this system. We have found that $2p_{\pm}$ states are not bounded for some values of the radius of the wire and of the applied magnetic field. We have shown that the applied magnetic field splits the degeneracy of the states with $n = 2$. Our theoretical results for the excitonic ground state compare quite well with some recent experimental reports. We believe our results are of importance in the quantitative understanding of future experimental work in this field.

Appendix

We consider a carrier of charge q in a cylindrical box of radius a, height b and dielectric constant ε. The carrier experiences a radial finite confinement potential $V(\rho)$ and an infinite confinement potential in the faces of the box. If the carrier is a hole, $q = +e$ and if it is an electron, $q = -e$. A uniform magnetic field is applied in the axial direction of the box. In the effective-mass approximation, the Hamiltonian of the carrier is expressed as

$$\boldsymbol{H} = \frac{1}{2m^*}\left[\boldsymbol{P} - \frac{q}{c}\boldsymbol{A}\right]^2 + \boldsymbol{V}(\rho) \tag{A1}$$

where the first term of equation (A1) is the carrier's kinetic energy in a magnetic field and the last term is the confinement potential in the radial direction. The vector potential is written as $\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2}(\boldsymbol{B} \times \boldsymbol{r})$ with $\boldsymbol{B} = B\underline{\boldsymbol{z}}$. In cylindrical coordinates, its components are

$$A_\rho = A_z = 0 \qquad A_\varphi = \tfrac{1}{2}(B\rho). \tag{A2}$$

On expanding the parenthesis of equation (A1), the Hamiltonian takes the form

$$\boldsymbol{H} = \frac{1}{2m^*}\left[\boldsymbol{P}^2 - \frac{q}{c}B\boldsymbol{L}_z + \frac{q^2}{c^2}\left(\frac{B^2\boldsymbol{\rho}^2}{4}\right)\right]^2 + \boldsymbol{V}(\rho) \tag{A3}$$

where $\boldsymbol{L}_z = -\mathrm{i}\hbar\partial/\partial\varphi$ in equation (A3) and the Hamiltonian is written as

$$\boldsymbol{H} = -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{\mathrm{i}q\hbar B}{2m^*c}\frac{\partial}{\partial\varphi} + \frac{q^2B^2\boldsymbol{\rho}^2}{8m^*c^2} + \boldsymbol{V}(\rho). \tag{A4}$$

In order to express the Hamiltonian in atomic units of length, $a_0 = \varepsilon\hbar^2/\mu e^2$, and of energy, $R^* = \hbar^2/2\mu a_0^2$, we define the lengths $\rho = \underline{\rho}a_0$ and $z = \underline{z}a_0$. In these units and in cylindrical coordinates the carrier's Hamiltonian is

$$\underline{\boldsymbol{H}} = \frac{\boldsymbol{H}}{R^*} = -\frac{\mu}{m}\underline{\nabla}^2 \mp \mathrm{i}\gamma\frac{\partial}{\partial\varphi} + \frac{m}{\mu}\frac{\gamma^2\underline{\boldsymbol{\rho}}^2}{4} + \boldsymbol{V}(\underline{\rho}). \tag{A5}$$

In this equation, γ is the energy of the carrier in a magnetic field in the first Landau level ($n = 0$), and is given by

$$\gamma = \frac{q\hbar B}{2mcR^*}. \tag{A6}$$

Expressing the Laplacian in cylindrical coordinates, equation (A5) is written in the following way:

$$\underline{\boldsymbol{H}} = -\frac{\mu}{m}\left[\frac{1}{\underline{\rho}}\frac{\partial}{\partial\underline{\rho}}\left(\underline{\rho}\frac{\partial}{\partial\underline{\rho}}\right) + \frac{1}{\underline{\rho}^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial\underline{z}^2}\right] \mp \mathrm{i}\gamma\frac{\partial}{\partial\varphi} + \frac{m}{\mu}\frac{\gamma^2\underline{\boldsymbol{\rho}}^2}{4} + \boldsymbol{V}(\underline{\rho}). \tag{A7}$$

The time-independent Schrödinger equation is $\underline{\boldsymbol{H}}\Psi = \underline{E}\Psi$, whose solutions can be written in a product form as $\psi(\underline{\rho}, \varphi, \underline{z}) = R(\underline{\rho}, \varphi)Z(\underline{z})$. In the time-independent Schrödinger equation, we substitute RZ for Ψ and divide the total equation by RZ, giving

$$-\frac{\mu}{m}\frac{1}{R}\frac{1}{\underline{\rho}}\frac{\partial}{\partial\underline{\rho}}\left(\underline{\rho}\frac{\partial R}{\partial\underline{\rho}}\right) - \frac{\mu}{m}\frac{1}{R}\frac{1}{\underline{\rho}^2}\frac{\partial^2 R}{\partial\varphi^2} \mp \frac{\mathrm{i}\gamma}{R}\frac{\partial}{\partial\varphi} + \frac{\mu}{m}\frac{\gamma^2\underline{\rho}^2}{4} + V(\underline{\rho}) - \underline{E} = \frac{\mu}{m}\frac{1}{Z}\frac{\mathrm{d}^2 Z}{\mathrm{d}\underline{z}^2}. \tag{A8}$$

The function Z is governed by the differential equation

$$\frac{\mu}{m}\frac{1}{Z}\frac{\partial^2 Z}{\partial\underline{z}^2} = -K^2 \tag{A9}$$

where $-K^2$ is a constant. It is demanded that $Z(z)$ is zero on the faces of the cylinder, $Z(-b/2) = Z(b/2) = 0$, which gives us the particular solution of equation (9),

$$Z(\underline{z}) = A\cos\left(\sqrt{\frac{m}{\mu}}K\underline{z}\right)$$

where $k = \pi n/b$, and $n = 1, 2, \ldots$. The differential equation for $R(\underline{\rho}, \varphi)$ is

$$-\frac{\mu}{m}\frac{1}{R}\frac{1}{\underline{\rho}}\frac{\partial}{\partial\underline{\rho}}\left(\underline{\rho}\frac{\partial R}{\partial\underline{\rho}}\right) - \frac{\mu}{m}\frac{1}{R}\frac{1}{\underline{\rho}^2}\frac{\partial^2 R}{\partial\varphi^2} \mp \frac{\mathrm{i}\gamma}{R}\frac{\partial R}{\partial\varphi} + \left(\frac{\mu}{m}\frac{\gamma^2\underline{\rho}^2}{4} + V(\underline{\rho}) - [\underline{E} - K^2]\right) = 0 \tag{A10}$$

with $\underline{E}_\rho = \underline{E} - K^2$. Substituting in this equation $r(\underline{\rho})\Phi(\varphi)$ for $R(\underline{\rho}, \varphi)$ and dividing by $r(\underline{\rho})\Phi(\varphi)$, we obtain for the total differential equation

$$-\frac{\mu}{m}\frac{1}{r}\frac{1}{\underline{\rho}}\frac{\partial}{\partial\underline{\rho}}\left(\underline{\rho}\frac{\partial r}{\partial\underline{\rho}}\right) - \frac{\mu}{m}\frac{1}{\Phi}\frac{1}{\underline{\rho}^2}\frac{\partial^2\Phi}{\partial\varphi^2} \mp \frac{\mathrm{i}\gamma}{\Phi}\frac{\partial\Phi}{\partial\varphi} + \left(\frac{\mu}{m}\frac{\gamma^2\rho^2}{4} + V(\underline{\rho}) - \underline{E}_\rho\right) = 0 \tag{A11}$$

where we have supposed that $\Phi(\varphi) = \mathrm{e}^{\mathrm{i}m\varphi}$, m being the eigenvalue of $\boldsymbol{L}_z$ in units of $\hbar$, in such a way that when Φ is substituted in equation (A11) and multiplied by $-r$ we obtain for the radial part of the differential equation

$$\frac{\mu}{m}\frac{1}{\underline{\rho}}\frac{\partial}{\partial\underline{\rho}}\left(\underline{\rho}\frac{\partial r}{\partial\underline{\rho}}\right) - \left(\frac{m^2}{\underline{\rho}^2} - m\gamma + \frac{m}{\mu}\frac{\gamma^2\underline{\rho}^2}{4} + V(\underline{\rho}) - \underline{E}_\rho\right)r = 0. \tag{A12}$$

With the purpose of expressing this differential equation in a well known form, we make the changes of variables

$$x = \frac{m}{\mu}\underline{\rho}^2 \qquad \mathrm{d}x = 2\underline{\rho}\frac{m}{\mu}\,\mathrm{d}\rho \qquad \frac{\partial r}{\partial\underline{\rho}} = \frac{\partial x}{\partial\underline{\rho}}\frac{\partial r}{\partial x} = 2\underline{\rho}\frac{m}{\mu}\frac{\partial r}{\partial x} \tag{A13}$$

with which we obtain the differential equation

$$4\frac{\partial}{\partial x}\left(x\frac{\partial r}{\partial x}\right) - \left(\frac{m^2}{x} - m\gamma + \frac{\gamma^2 x}{4} + V(x) - \underline{E}_\rho\right)r = 0. \tag{A14}$$

The solution suggested for $r(x)$ is

$$r(x) = \mathrm{e}^{-\beta x}x^{|m|/2}\chi(x). \tag{A15}$$

After some simplifications we obtain for this differential equation

$$4x\frac{\partial^2\chi}{\partial x^2} + 4(1 + |m| - 2\beta x)\frac{\partial\chi}{\partial x} + \left(\begin{array}{c} 4\beta^2 x - 4\beta - 4\beta|m| + m\gamma - \dfrac{\gamma^2 x}{4} \\ -V(x) - \underline{E}_\rho \end{array}\right)\chi = 0. \tag{A16}$$

In order to determine β we choose

$$4\beta^2 x - \frac{\gamma^2 x}{4} = 0 \tag{A17}$$

which gives

$$\beta = \frac{|\gamma|}{4}. \tag{A18}$$

With this done, and with the change of variable

$$y = \frac{\gamma x}{2} \tag{A19}$$

we obtain the differential equation whose solutions are the confluent hypergeometric functions $F(a_{|m|j}, b, y)$:

$$y\frac{\partial^2 F}{\partial y^2} + (1 + |m| - y)\frac{\partial F}{\partial y} - \left[\frac{1}{2}(1 + |m|) \pm \frac{m}{2} + \frac{(V(y) - \underline{E}_{\underline{\rho}})}{2\gamma}\right] F(y) = 0. \tag{A20}$$

Expressed in a concise way, equation (A20) takes the form

$$y\frac{\partial^2 F}{\partial y^2} + (b - y)\frac{\partial F}{\partial y} - aF(y) = 0. \tag{A21}$$

In equation (A20) the sign + (−), in the term $\pm m/2$, corresponds to the electron (hole). If the carrier is inside the box, the solution of equation (A20) is the confluent hypergeometric function $1F1(a_{|m|j,int}, b, y)$, where $a_{|m|j}$ corresponds to the state with magnetic quantum number $|m|$; otherwise, if the carrier is outside, the solution is the confluent hypergeometric function $U(a_{|m|j,ext}, b, y)$. Comparing (A20) and (A21) we found that $b = 1 + |m|$ and $a_{|m|j}$ are given by

$$\begin{aligned} a_{|m|j,ext} &= \frac{V - \underline{E}_{\underline{\rho}}}{2\gamma} + \frac{1}{2} + \frac{|m|}{2} \pm \frac{m}{2} \\ a_{|m|j,int} &= -\frac{\underline{E}_{\underline{\rho}}}{2\gamma} + \frac{1}{2} + \frac{|m|}{2} \pm \frac{m}{2} \\ a_{|m|j,ext} - a_{|m|j,int} &= \frac{V}{2\gamma}. \end{aligned} \tag{A22}$$

For example, the $a_{|m|j}$ are

$$\begin{aligned} a_{|m|j,ext} &= \frac{V - \underline{E}_{\underline{\rho}}}{2\gamma} + \frac{1}{2} + \frac{|m|}{2} + \frac{m}{2} \\ a_{|m|j,ext} &= \frac{V - \underline{E}_{\underline{\rho}}}{2\gamma} + \frac{1}{2} + \frac{|m|}{2} - \frac{m}{2} \end{aligned} \tag{A23}$$

for the electron and hole, respectively.

The energy eigenvalues of the carrier wave function are determined by the continuity of the wave functions and of its first derivative at the boundaries:

$$\begin{aligned} &\Psi_{int}(\underline{\rho}, \varphi, \underline{z})|_{\underline{\rho}=\underline{a}} = \Psi_{ext}(\underline{\rho}, \varphi, \underline{z})|_{\underline{\rho}=\underline{a}} \\ &\left.\frac{\partial \Psi_{int}(\underline{\rho}, \varphi, \underline{z})}{\partial \underline{\rho}}\right|_{\underline{\rho}=\underline{a}} = \left.\frac{\partial \Psi_{ext}(\underline{\rho}, \varphi, \underline{z})}{\partial \underline{\rho}}\right|_{\underline{\rho}=\underline{a}}. \end{aligned} \tag{A24}$$

If the radial confinement potential is infinite, the value of $a_{|m|j,int}$ is determined by the boundary condition for which the wave function is equal to zero at the surface of the box, $\underline{\rho} = \underline{a}$, $1F1(a_{|m|j}, 1 + |m|, \xi_{\underline{a}}) = 0$, where j is the jth zero of the confluent hypergeometric

function and $\underline{a} = a/a_0$. Knowing the value of $a_{|m|j,int}$, it is replaced in equation (A22) and the energy of the carrier is determined by means of

$$\underline{E}_{\underline{a}} = 2\gamma \left(-a_{|m|j} + \frac{1}{2} + \frac{|m|}{2} \right). \tag{A25}$$

The E_{01} energy of the carrier is found by setting $m = 0$ in $a_{|m|j,int}$, where j is the first zero of the carrier's confluent hypergeometric function, and is given by

$$\underline{E}_{01} = \gamma(1 - 2a_{01}). \tag{A26}$$

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