Lighthole exciton in cylindrical microtube with two quantum wells

J D González1,2, J E Gonzalez3, J Barba-Ortega2

1 Grupo Teoría de la Materia Condensada, Universidad del Magdalena, Santa Marta, Colombia.
2 Departamento de Física, Facultad de Ciencias, Universidad Nacional de Colombia, Bogotá.
3 Escuela de Física, Universidad Industrial de Santander, Bucaramanga, Colombia

E-mail: jedgonzalezac@unal.edu.co

Abstract. We report on microtube with double quantum well and large radius of curvature. Method for calculating the ground-state energy of light hole exciton and density of states confined in a square potential model that consist of a narrow well, which is produced by a symmetrical structure. The exciton trial function is taken as a product of the ground state wave functions of both the unbound electron and hole in the heterostructure, with an arbitrary correlation function that depends only on electron-hole separation. A renormalized Schrödinger equation for the correlation function is derived and coincides with the corresponding equation for a hydrogen atom in an effective and space-isotropic homogeneous. The binding energy of the ground state to an exciton in this heterostructure, the contribution to the energy given by the sublevels and the density of states is determined as a function of the width of the well, the aluminum concentration and confinement potential profile is obtained by solving the equation calculated by the variational model proposed.

1. Introduction

The progress in nanoscale technology has made possible the fabrication of low-dimensional heterostructures with controlled thickness and relatively sharp interfaces, where the excitons remain present even at room temperature because of the quantum confinement increases highly the electron–hole attraction [1]. A great deal of attention has been devoted to experimental studies of excitons in heterostructures based on III–V semiconductor [2–8] particularly quantum wells (QWs), superlattices (SLs), quantum-well wires (QWWs), quantum dots (QDs), quantum rings (QRs) and more recently microtube [9]. The multilayer structures including strained layers are useful to form nanotubes and nanocoils [10]. By using lattice-mismatched epitaxial layers that rolled up when freed from the substrate [11-13] due to the built-in strain and a micro-tube including two GaAs/GaAlAs quantum wells (QWs) [14,15] located at positions with different types of strain was fabricated and its optical properties before and after the fabrication process were investigated by photoluminescence (PL) spectroscopy [16]. The purpose of this paper is to analyze the density of the states of a light-hole exciton as a function of the width of quantum wells taking into account the ground state energy and the contribution given by sublevels in a microtube with two GaAs/AlGaAs quantum wells.
Throughout the heterostructures [10]. In this case the characteristic energy of an exciton can consequently be defined through the effective Rydberg $R_\theta^e = e^2 / 2 e a_0^\ast$, and its characteristic length through the effective Bohr radius, $a_\theta^e = \varepsilon \hbar / \mu e^2$, with $\mu = m_e^* m_h^* / (m_e^* + m_h^*)$ being the reduced exciton effective mass. Thus the dimensionless Hamiltonian for the electron-hole pair confined in a heterostructure in the presence of an external field may be written as:

$$H(r_e, r_h, \tau) = H_e(r_e) + H_h(r_h) + V(r_e, r_h) - 2\tau / r_{eh} \quad (\tau = 0, 1)$$

$$H_e = -\eta_e \nabla_e^2 + V_e(r_e); \quad H_h = -\eta_h \nabla_h^2 + V_h(r_h)$$

Where $H_e$ and $H_h$ describe the free motion of electron and hole confined in the heterostructure respectively, $V(r_e, r_h)$ is a potential confinement, $-2/r_{eh}$ is the energy of the electron-hole interaction, $r_e$ and $r_h$ are electron and hole position vectors, and $r_{eh} = |r_e - r_h|$ is the electron-hole separation. The parameter $\tau$ in Eq.(1) is equal to 1 for exciton and to 0 for uncorrelated electron-hole pair, and the parameters $\eta_e = \mu / m_e^*$ and $\eta_h = \mu / m_h^*$ in Eq.(4) are characteristics of the corresponding dimensionless effective masses of the hole in units of the reduced exciton effective mass $\mu$ respectively. For an uncoupled electron-hole pair ($\tau = 0$), the Hamiltonian is separable, on the contrary for exciton ($\tau = 1$), and the Schrödinger equation can only be solved by using some approximation methods. Assuming that the center of mass motion is affected by the electron-hole interaction to a considerably smaller degree than the relative motion, we choose the ground state exciton trial function in the form:

$$\Psi(r_e, r_e) = f_0(r_e, r_h) \Phi(r_{eh}); \quad r_{eh} = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2 + (z_e - z_h)^2}$$

where $f_0(r_e, r_h)$ is the product of the one-particle electron and hole ground state wave functions, whereas $\Phi(r_{eh})$ is a variational function that describes the intrinsic properties of the exciton and depends only on the electron-hole separation. The ground state energy of the exciton is found by minimizing the functional, after some algebraic manipulations we can obtain the following variational problem:

$$F[\Phi] = \int_0^\infty \left\{ f_0(r) \left[ \left( \frac{d\Phi(r)}{dr} \right)^2 + (E_0 - E_{ex} - \frac{2}{r}) \right] \Phi^2(r) \right\} dr \to \text{min}$$

with $E_0 = E_e + E_h$ being the ground state energy of the uncoupled electron-hole pair, $r = r_{eh}$ and

$$f_0(r) = \int d r_e \int f_0^2(r_e, r_h) \delta(|r_e - r_h| - r) d r_h$$

The minimization of the functional (6) with respect to $\Phi$ and its first derivative yields the Euler-Lagrange equation

$$\frac{1}{f_0(r)} \frac{d}{dr} f_0(r) \frac{d\Phi(r)}{dr} - \frac{2}{r} \Phi(r) = [E_{ex} - E_0] \Phi(r)$$

The binding energy of the exciton, $E_b = E_0 - E_{ex}$, is then obtained by solving numerically Eq. (8).
\[ E_i(m) = \Delta_i + \frac{m^2}{R_i^2}; \quad \Delta_i = E_g + E_x (\omega_i) \]  
(9)

Here \( E_g \) is the gap between the valence and the conduction bands for the material of the QW. All energies are taken to be referred to the top of the valence band equal to zero. In order to calculate the density of the energy states (DOS) with respect to the valence band to excitonic state transition we assume that the resulting DOS is an envelope curves of all individual transitions

\[ \rho(E) = \sum_{\Delta} \sum_{m=0.1} \int (E - E_i(m)) f(x) = \frac{1}{\sigma^{\sqrt(2\pi)}} \exp(-x^2/2\sigma^2) \]  
(10)

3. Results and Discussion

In Fig. 2 We compare the binding energies of the light-hole exciton as a function of the width \( L \) of the cylindrical microtube GaAs/Ga\( _{0.7}\)Al\( _{0.3}\)As for different potential shapes Figure 1, with those previously obtained by Greene, Bajaj and Phelps [2]. In this calculation we intentionally chose the material parameters that roughly correspond to those from Ref. 2. The excellent agreement observed in all cases suggests that we can obtain novel curves for different configurations of the heterostructure.

In Fig. 3. Shows that the peaks position of the density of states of light hole exciton are inverted due to peaks with longer wavelengths have less energy according to the equation \( \lambda = \frac{1242}{E_{exc}} \). As we can see the behavior of excitonic states density is similar to that obtained by photoluminescence curve ref. [9], high coincidence of peaks corresponding to wavelengths in both curves is shown, by taking the well width 0.2\( a_0 \) and 0.3\( a_0 \). Moreover, the difference in the height of the peaks in Figure 2. is due to the choice in the location of wells QW2 and QW1, for radii \( R_1 \) and \( R_2 \) in the microtube. The higher peaks in the QW’s is located in the position corresponding to the value of \( R \) with smaller radius of curvature.
Figure 3. Curves of light-hole density states as a function of a). exciton energy and b). Wavelength in a microtube with two rectangular quantum well.

3. Conclusion
The executed numerical simulations show the binding energy behavior for the lowest state of the light-hole in a microtube with two wells with rectangular and soft barriers, taking into account the sublevels due to the rotational kinetic energy. We found that our calculations are in a good agreement with experimental case. Also we present new curves that show novel density of states peaks and different configurations of a microtube can be analyzed.

Acknowledgement
This work was partially financed by the Universidad Del Magdalena and the Colombian Agency COLCIENCIAS through doctoral scholarships 567.

4. References
[1] Miller D A 1988 in: H. Hang, L. Banyai (Eds.), Optical Switching in Low-Dimensional Systems, Plenum, New York, pp. 1–8.
[2] Greene R L, Bajaj K K, Phelps D E 1984 Phys. Rev. B 29 1807.
[3] Cen J, Bajaj K K, 1992 Phys. Rev. B 46 15280; Cen J, Bajaj K K, 1994 Phys. Rev. B 50 g10947.
[4] Gang Li, Branis S V, Bajaj K K, 1995 J. Appl. Phys. 77 1097.
[5] Goff S Le, Stebe B, 1993 Phys. Rev. B 47 1383.
[6] Garm T, J. 1996 Condens. Matter. 8 5725.
[7] Ferreyra J M, Proetto C R, 1998 Phys. Rev. B 57 9061; Bolcatto P G, Proetto C R, 1999 Phys. Rev. B 59 12487.
[8] Glutsch S, Bechstedt F, Wegscheider W, Schedelbeck F, 1997 Phys. Rev. B 56 4108.
[9] Kubota K, Vaccaroa P O, Oltania N, Hiroseb Y, Hosodab M, Aida T, 2002 Physica E 13 313–316.
[10] Prinz V Ya, Selezniev V A, Samoylov V A, Gutakovsky A K, 1996 Microelectron. Eng. 30 439.
[11] Lao Y F, 2010 Applied Physics Letters 97, 091104.
[12] Rodriguez R D, Nanoscale Research Letters, 2012 7, 594.
[13] Balkhorn F, Mansfeld S, Krohn A, Topp J, Hansen W, Heitmann D, Mendach S, Phys Rev Lett, 104 (3):037205. (2010).
[14] Miranda G L, Mora-Ramos M E, Duque C A, 2013 Physica B 409 78–82.
[15] Syrbu N, Dorogan A, Dragutan N, Vieru T, Ursaki V, 2011 Physica E 44, 202–206.
[16] Nakayama M, Hirao T, Hasegawa T, 2010 Physica E 42, 2644–2647.