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Density of states for a light-hole exciton in a microtube of GaAs/AlGaAs with two quantum well and different potential shape: theoretical model

A D Barrios[1] J. Barba-Ortega[2] and J D González[1,2]
[1] Grupo Teoría de la Materia Condensada, Universidad del Magdalena, Santa Marta, Colombia.
[2] Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia.

E-mail: jedgonzalezac@unal.edu.co

Abstract. We consider a simple method for calculating the ground-state energy of light hole exciton and density of states confined in a microtube of GaAs/AlGaAs recently fabricated and studied experimentally, with a double quantum well and large radius of curvature. 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 aluminium concentration and confinement potential profile is obtained by solving the equation calculated by the variational model proposed.

1. Introduction

It is well known that 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.

2. Theory

We propose a simple variational procedure in which the problem of a light-hole exciton in a microtube with two $GaAs/Ga_{1-x}Al_xAs$ quantum wells (QWs) is considered as we can see in the figure 1 (a). For modelling a microtube, we use the confinement potential figure 1 (b) given by the following expression:

$$V(z) = V_0\theta(-z, -L/2, W) + V_0\theta(z, L/2, W) \tag{1}$$

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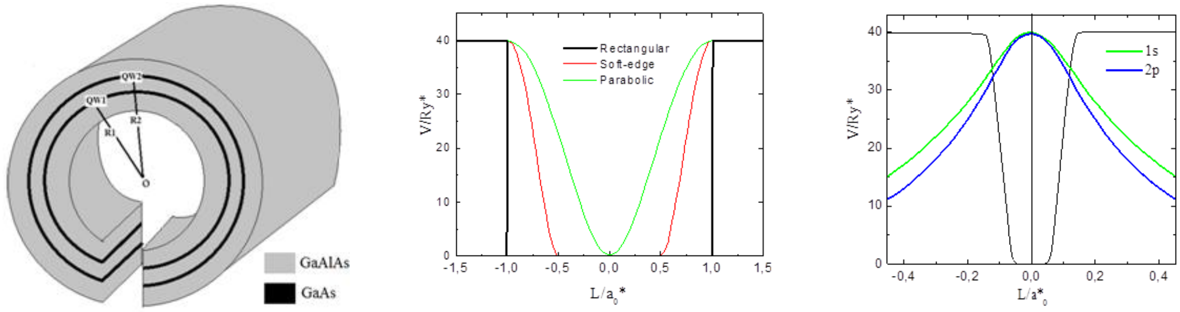
$$\theta(z, z_0, W) = \begin{cases} 0; & z < z_0 - W \\ [(z - z_0)^2/W^2 - 1]^2 \; ; & z_0 - W \le z < z_0 \\ 1; & z \ge z_0 \end{cases} \qquad (2)$$

The wave function of the free electron and light-hole is Shown in the figure 1 (c). The strong confinement due to the narrow quantum well used, shows a mixing of the wave functions and strong penetration in the bulk.



(a) **(b)** **(c)**

Figure 1. (a) Cylindrical microtube, containing two GaAs/GaAlAs quantum wells (QWs). (b) Potential shape with different widths of the transition region. (c) Waves functions of the electron ground 1s and the first excited 2p for a light-hole exciton.

In this work, we consider a single exciton in semiconductor heterostructures within the effective mass approximation by using an spherical hole mass approximation and constant physical parameters throughout the heterostructures [10]. In this case the characteristic energy of an exciton can consequently be defined through the effective Rydberg $R_y^* = e^2\ /2\varepsilon\, a_0^*$, and its characteristic length through the effective Bohr radius, $a_0^* = \varepsilon\hbar/\mu e^2$, 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:

$$H(\boldsymbol{r}_e, \boldsymbol{r}_h, \tau) = H_e(\boldsymbol{r}_e) + H_h(\boldsymbol{r}_h) + V(\boldsymbol{r}_e, \boldsymbol{r}_h) - 2\tau/r_{eh} \qquad (\tau = 0{,}1) \qquad (3)$$

$$H_e = -\eta_e \nabla_e^2 + V_e(\boldsymbol{r}_e);\ H_h = -\eta_h \nabla_{\square}^2 + V_{\square}(\boldsymbol{r}_{\square}) \qquad (4)$$

Where H_e and H_h describe the free motion of electron and hole confined in the heterostructure respectively, $V(\boldsymbol{r}_e, \boldsymbol{r}_h)$ is a potential confinement, $-2/r_{eh}$ is the energy of the electron-hole interaction , $\boldsymbol{r}_e$ and $\boldsymbol{r}_e$ are electron and hole position vectors, and $r_{eh} = |\boldsymbol{r}_e - \boldsymbol{r}_h|$ is the electron-hole separation. The parameter τ in equation (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 equation (4) are characteristics of the corresponding dimensionless effective masses of the hole in units of the reduced exciton effective mass μ 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:

$$\Psi(\boldsymbol{r}_e, \boldsymbol{r}_e) = f_0(\boldsymbol{r}_e, \boldsymbol{r}_h)\Phi(r_{eh});\ r_{eh} = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2 + (z_e - z_h)^2} \qquad (5)$$

where $f_0(\boldsymbol{r}_e, \boldsymbol{r}_h)$ 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 variation problem:

$$F[\Phi] = \int_0^\infty \left\{ J_0(r) \left[\left(\frac{d\Phi(r)}{dr} \right)^2 + \left(E_0 - E_{ex} - \frac{2}{r} \right) \right] \Phi^2(r) \right\} dr \ \rightarrow min \tag{6}$$

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

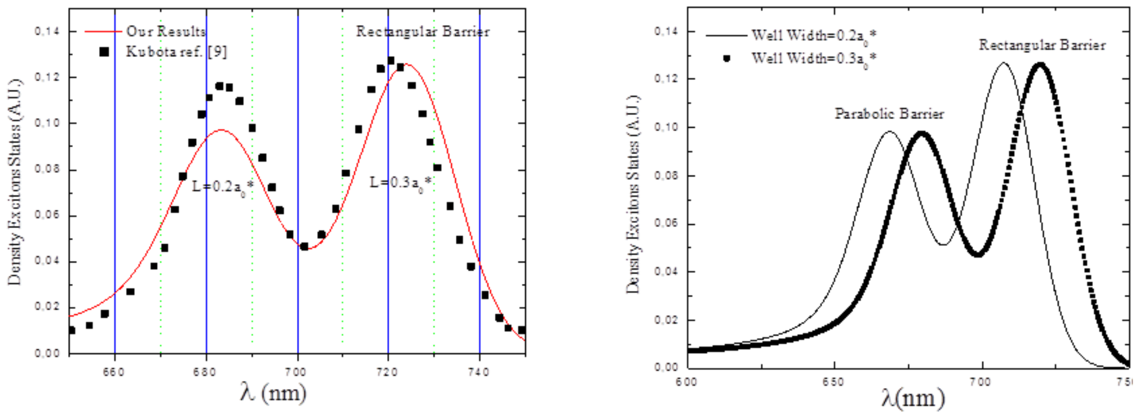
$$J_0(r) = \int d\boldsymbol{r}_e \int f_0^2(\boldsymbol{r}_e, \boldsymbol{r}_h) \delta(|\boldsymbol{r}_e - \boldsymbol{r}_h| - r) d\boldsymbol{r}_h \tag{7}$$

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

$$\frac{1}{J_0(r)} \frac{d}{dr} J_0(r) \frac{d\Phi(r)}{dr} - \frac{2}{r} \Phi(r) = [E_{ex} - E_0] \Phi(r) \tag{8}$$

The binding energy of the exciton, $E_b = E_0 - E_{ex}$, is then obtained by solving numerically equation (8). In the figure 2 the inclusion of the two quantum wells is reflected in the curves of density of excitonics states in microtube. The energy of sublevels are obtained including the contribution the rotational kinetic energy which is added to the exciton energy and gap, may be written as:

$$E_i(m) = \Delta_i + \frac{m^2}{R_i^2} \tag{9}$$



(a) **(b)**

Figure 2. Shift in the peak position in the state density curve in function of the wavelength for different shapes of the confinement potential.

Where $i = 1,2$, Δ_i is the exciton energy plus the gap energy, m magnetic quantum number and R_i radii from center of microtube since QW1 or QW2 figure1 (b). figure 2. Shows the density of states for a light-hole exciton in a microtube, with radii $R_1 = 2.5a_0^*$ $R_2 = 5.7a_0^*$ corresponding to the width of the well $L_1 = 3nm = 0.3a_0^*$ y $L_2 = 2nm = 0.2a_0^*$ respectively. This graph shows that the behavior of excitonic states density is similar to that shown by photoluminescence curve ref. [9], high coincidence of peaks corresponding to wavelengths in both curves is shown. Moreover, the difference in the height of the peaks in figure 2 (a) and (b). 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. figure1 (b) shows additional confinement produced by interdiffusion $Ga_{1-x}Al_xAs$ material into the well in GaAs, while figure 2 (b) shows the achieved energy due to the interdiffusion, in each well and hence in the position of each peak. We see higher energy values are achieved by using smaller well widths. Additionally, the parabolic profile provides a higher potential than the rectangular profile confinement. Figure 2 (a) The curve measured experimentally by photoluminescence [9] is compared with the energy density of states of a light hole exciton with square well profile and radius of the first well QW1, $\mathrm{R_1} = 2.5\mathrm{a}_0^*$ and radius of the second well QW2, $\mathrm{R_2} = 5.7\mathrm{a}_0^*$.

3. Conclusions
We have presented a simple method of calculation of the binding energy for the lowest state of the light-hole in a microtube with two wells with different potential shapes, taking into account the sublevels due to the rotational kinetic energy. We found that ours calculus are in a good agree with experimental case. Also we present new curves that show novels density of states peaks and different configuration of a microtube can be analyzed.

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