Physica B 511 (2017) 68–73

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Non-linear optical response of an impurity in a cylindrical quantum dot under the action of a magnetic field

Alfonso A. Portacio[a,*], Boris A. Rodríguez[b], Pablo Villamil[c]

[a] Universidad de los Llanos, Departamento de Matemáticas y Física, Facultad de Ciencias básicas e Ingenierías, Villavicencio, Colombia
[b] Instituto de Física, Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín, Colombia
[c] Universidad de Sucre, Departamento de Física, Facultad de Educación y Ciencias, Sincelejo, Colombia

ARTICLE INFO

Keywords:
Cylindrical quantum dot
Binding energy
Donor impurity
Nonlinear optical
Optical rectification
Refractive index
Optical absorption

ABSTRACT

The linear and nonlinear optical response in a cylindrical quantum dot (CQD) of $GaAs/Ga_{0.6}Al_{0.4}As$ with a donor impurity in a uniform magnetic field applied in the axial direction of the cylinder is studied theoretically. The calculations were carried out in approximations of effective mass and two-level quantum systems. Using the variational method, the binding energies and the wave functions of the 1s-like y 2pz-like states for different positions of the impurity inside the CQD were found. It was found that the binding energy is greatest in the center of the CQD and diminishes as the impurity moves radially and/or axially. The optical rectification, the change in the refractive index, and the optical absorption were studied as functions of the energy of a photon incident on the CQD and different intensities of the magnetic field, with an impurity located at various positions. It was found that in a CDQ with an impurity inside, the effect of the variation of the intensity of the magnetic field on the optical response is much less than the effect produced by the variation of the position of the impurity. The physical reason for this behavior is that in nanostructures with impurities the Coulomb confinement is stronger than the magnetic confinement. It was also found that when the impurity is in the center of the quantum dot, the optical rectification coefficient is zero, due to the symmetry that the wave function of the impurity exhibits at this geometric point. When the impurity moves in the axial direction, the symmetry is broken and the optical rectification coefficient is different from zero, and its value increases as the impurity moves away from the center of the CQD.

1. Introduction

Recent advances in the nanotechnology of semiconductors have allowed designing and producing a great variety of low-dimensional quantum systems, such as quantum wells, quantum wires, and quantum dots (QDs) [1], which have contributed to the evolution of nanoelectronics and the development of technologies such as laser production, sources of photon emission, quantum clocks, and some technologies applicable to quantum information, quantum computing, etc. [2,3]. Nevertheless, QDs are the most-explored nanostructures, because the tridimensional confinement of the charge carriers leads to the formation of energy spectra similar to those that are exhibited in atomic systems. These discrete levels of energy can be adjusted by means of the control of the size of the QDs and/or the action of external agents such as temperature, hydrostatic pressure, electrical fields, and magnetic fields, etc. [4]. Theoretical and experimental research can be found in the literature that studies the optical properties of QDs with varying geometry and dimensions for application in non-linear optical devices. Some research uses cylindrical quantum dots to study non-linear optical phenomena such as optical rectification [5], generation of the second harmonic [6], generation of the third harmonic [7], and changes in the index of refraction and the optical absorption [8].

On the other hand, when impurity atoms are added to nanostructures, the number of charge carriers in the nanostructure changes, producing changes in the optical and electronic properties of these low-dimensional systems. For this reason, the properties of the impurities in nanostructures are an object of study by diverse authors. Ribeiro and Latgé [9] carried out a comparative study of impurities in QDs and investigated the binding energy and the density of states of a donor impurity within a cylindrical QD and a spherical QD, finding that for volumes equal to the binding energy and the form of the density of states they don't depend on the geometry of the nanostructured quantum system. The effect of a magnetic field on the binding energy of donor impurities in quantum wires [10–12] and in QDs [13–15] has also been reported. These investigations show that only for the 1s-like state does the binding energy increase approximately linearly with the

* Corresponding author.
E-mail address: aportacio@unillanos.edu.co (A.A. Portacio).

http://dx.doi.org/10.1016/j.physb.2017.02.008
Received 31 December 2016; Received in revised form 1 February 2017; Accepted 7 February 2017
Available online 08 February 2017

applied magnetic field. With respect to the nonlinear optical response in nanostructures, the effect that impurities have on optical rectification [16], the change in the refractive index [17], the optical absorption [18], and the generation of harmonics [19,20] have been investigated, and it has been concluded that the presence of impurities in quantum systems: i) increases the difference in energy between the subbands, and therefore the resonance peaks undergo a blue shift; ii) reduces the transition matrix elements, causing a decrease in the magnitude of the optical properties.

In the present article, a theoretical study of the linear and nonlinear optical response generated by the interaction between a classical optical field and a CQD of $GaAs/Ga_{0.6}Al_{0.4}As$ with a donor impurity subjected to the action of a uniform magnetic field applied in the axial direction of the cylinder is presented. Furthermore, the effect of the magnetic field and the position of the impurity within the CQD on the binding energy, the optical rectification, the change in the refractive index, and the optical absorption is analyzed.

This article is organized in the following way: in Section 2 the theory used for finding the above-described magnitudes is presented. In Section 3, the analytical and numerical results and their analysis are presented, and in Section 4 we present our conclusions.

2. Theoretical background

2.1. Characteristic values of the energy and of the characteristic functions of the system

The system under study consists of a donor impurity confined in a CQD in the presence of a uniform magnetic field $\boldsymbol{B}$ oriented in the axial direction of the CQD. Within the framework of the effective mass approximation, the Hamiltonian $\hat{H}_0$ of the impurity is [11,21]:

$$\hat{H}_0=\frac{1}{2\ m^*}\left(\hat{\boldsymbol{P}}-\frac{e}{c}\boldsymbol{A}\right)^2-\frac{e^2}{\varepsilon|\boldsymbol{r}-\boldsymbol{r_0}|}+V_{conf}(\boldsymbol{r}), \tag{1}$$

where $|\boldsymbol{r}-\boldsymbol{r_0}|=\sqrt{(\rho-\rho_0)^2+(z-z_0)^2}$, $\boldsymbol{r_0}$ is the position of the impurity measured from the center of the CQD, ε is the dielectric permittivity of the nanostructure, m^* is the effective mass of the electron, $\hat{\boldsymbol{P}}$ is the linear moment operator, e is the charge of the electron, c is the speed of light in a vacuum, $\boldsymbol{A}$ is the potential vector of the uniform magnetic field, which can be written as $\boldsymbol{A}(\boldsymbol{r})=\frac{1}{2}\boldsymbol{B}\times\boldsymbol{r}$ with $\boldsymbol{B}=B\hat{z}$ and which in cylindrical coordinates is converted into $A_\rho=A_z=0$, and $A_\varphi=\frac{1}{2}B\rho$, $V_{conf}(\boldsymbol{r})$ is a potential of finite confinement, defined as follows:

$$V_{conf}(\boldsymbol{r})=V_{conf}(\rho,\varphi,z)=V_\rho(\rho)+V_z(z), \tag{2}$$

where

$$V_\rho(\rho)=\begin{cases}V_0\left(\frac{\rho}{R}\right)^2, & \rho\le R\\ V_0, & \rho>R\end{cases} \tag{3}$$

$$V_z(z)=\begin{cases}0, & |z|\le\ \frac{L}{2}\\ V_0, & |z|>\ \frac{L}{2}\end{cases} \tag{4}$$

R and L are the radius and the length of the cylinder, respectively.

Using cylindrical coordinates and reduced atomic units, the following magnitudes are determined: effective Bohr radius, $a^*=\frac{\hbar^2\varepsilon}{m^*e^2}$ for the length and Rydberg, $R^*=\frac{m^*e^4}{2\hbar^2\varepsilon^2}$ for the energy. Now (1) can be written in the form:

$$\hat{H}_0(\rho,\phi,z)=\hat{H}(\rho,\phi)+\hat{H}(z)-\frac{2}{\sqrt{(\rho-\rho_0)^2+(z-z_0)^2}}, \tag{5}$$

where

$$\hat{H}(\rho,\phi)\psi_1(\rho,\phi)=\left[-\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)-\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}-i\gamma\frac{\partial}{\partial\phi}+\frac{1}{4}\gamma^2\rho^2+V_\rho(\rho)\right]\psi_1(\rho,\phi)=E_1\psi_1(\rho,\phi), \tag{5.1}$$

$$\hat{H}(z)\psi_2(z)=\left[-\frac{d^2}{dz^2}+V_z(z)\right]\psi_2(z)=E_2\psi_2(z). \tag{5.2}$$

Eqs. (5.1) and (5.2) represent the Schrödinger equations independent of time in the radial and axial directions from the quantum dot. $\gamma=\frac{e\hbar B}{2m^*cR^*}$ is an adimensional measure of the magnetic field. The solution of (5.1) is known [11,22], and is given by:

$$\psi_1(\rho,\phi)=N_1\begin{cases}e^{-\beta_1R^2}1F1(a_i,1+m,2\beta_1\rho^2)e^{im\phi}, & \rho\le R\\ e^{(\beta_2-\beta_1)R^2}\frac{1F1(a_i,1+m,2\beta_1R^2)}{1U1(a_e,1+m,2\beta_2R^2)}1U1(a_e,1+m,2\beta_2\rho^2)e^{im\phi}, & \rho\ge R\end{cases} \tag{6}$$

where $\beta_1=\frac{\sqrt{4V_0+(\gamma R)^2}}{4R}$, $\beta_2=\frac{\gamma}{4}$, $a_i=\frac{1}{2}-\frac{E_1}{8\beta_1}$, $a_e=\frac{1}{2}-\frac{(E_1-V_0)}{8\beta_2}$, m is the magnetic quantum number, and N_1 is the normalization constant. $1F1(a,b,x)$ and $1U1(a,b,x)$ are confluent hypergeometric functions. Applying boundary conditions to the wave functions described in (6), one obtains the transcendental equation that determines the values of the energy E_1 for each m. The solution for (5.2) is also known [23], and for the ground state it has the following expression:

$$\psi_2(z)=N_2\begin{cases}e^{k_2\left(\frac{L}{2}+z\right)}Cos\left(k_1\frac{L}{2}\right), & z<-\frac{L}{2},\\ Cos(k_1z), & -\frac{L}{2}<z<\frac{L}{2}\\ e^{k_2\left(\frac{L}{2}-z\right)}Cos\left(k_1\frac{L}{2}\right), & z>\frac{L}{2}\end{cases} \tag{7}$$

$k_1=\sqrt{E_2}$, $k_2=\sqrt{V_z(z)-E_2}$. The value of the energy E_2 is determined by solving Eq. (8).

$$Tan\left(k_1\frac{L}{2}\right)=\frac{k_2}{k_1}. \tag{8}$$

In order to calculate the impurity energy in the CQD for the $1s$-like and $2Pz$-like states, the variational method is used [24], taking the following test functions:

$$\Psi_{1s}(\rho,\phi,z)=N_{1s}\psi_1(\rho,\phi)\psi_2(z)\Gamma_{1s}(r,\lambda_{1s}), \tag{9}$$

$$\Psi_{2Pz}(\rho,\phi,z)=N_{2Pz}\psi_1(\rho,\phi)\psi_2(z)\Gamma_{2Pz}(r,\lambda_{2Pz}), \tag{10}$$

where $m=0$ for $\psi_1(\rho,\phi)$ and N_{1s} and N_{2Pz} are constants of normalization. The functions $\Gamma_{1s}(r,\lambda_{1s})$ and $\Gamma_{2Pz}(r,\lambda_{2Pz})$ are hydrogenic orbitals for the $1s$-like and $2Pz$-like states, respectively, detailed in Ref. [25]. λ_{1s} and λ_{2Pz} are variational parameters that are obtained by minimizing the expected value of the Hamiltonian described in (5), and correspond to the impurity energy, that is:

$$E^x_{imp}=\left(\frac{\langle\Psi_x(\rho,\phi,z)\hat{H}\Psi_x(\rho,\phi,z)\rangle}{\langle\Psi_x(\rho,\phi,z)|\Psi_x(\rho,\phi,z)\rangle}\right)_{min(\lambda_x)} \tag{11}$$

where E^x_{imp} is the impurity energy in the CQD for state x.

The binding energy $E_{b,x}$ of a hydrogenic impurity is the energy necessary to move its electron from state x of the impurity to the first level of the conduction subband. The calculation of the binding energy is carried out by means of the application of (12) [11]:

$$E_{b,x}=E_0-E^x_{imp}, \tag{12}$$

where $E_0=E_1+E_2$ corresponds to the energy of the first level of the conduction subband of the quantum dot CQD of $GaAs/Ga_{1-x}Al_xAs$ with a uniform magnetic field applied in the axial direction of the cylinder.

2.2. Linear and nonlinear optical response

In this section, a brief derivation of the optical response that a