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Magneto-optical properties in inhomogeneous quantum dot: The Aharonov-Bohm oscillations effect

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ABSTRACT

In this study, we investigated theoretically the effect of a magnetic field B on the linear, nonlinear, and total absorption coefficients (ACs) and the refractive index changes (RICs) associated with intersubband transitions in the HgS quantum shell. In the calculations, a diagonalization method was employed within the effective-mass approximation. We find that a three kinds of optical transitions (S–P, P–D and D–F) between the ground state and the first excited state appear, resulting from the oscillation of the ground state with B (Aharonov-Bohm effect). In the other hand, the magnetic field enhances and diminishes their related RICs and ACs intensities respectively for the three kinds of optical transitions, and shifts their peaks towards low energy (blue shift).

1. Introduction

The core shell quantum dot (CSQD) represents the newest trend in nanocrystal research, due to their promising optoelectronic properties [1]. In the other hand the field of nonlinear optics of low-dimensional materials (core shell quantum dots) continued to achieve new advances both in fundamental physics and in practical applications such as electronic and optoelectronic devices in the infrared region of electromagnetic spectrum.

Recently, particular attention has been devoted to the investigation of the optical properties of the inhomogeneous core shell spherical quantum dot taking into account the finite barrier potential model. For example P. Christina lily Jasmine et al. investigated the optical properties using the density matrix approach. They showed that the absorption can be tuned by varying the size and the material composition of the core shell quantum dot [2]. Niculescu and. Cristea studied the effect of the dielectric mismatch between the core shell and the surrounding material on the optical properties [3,4]. Also the optical properties in a CdSe/$Pb_{1-x}Cd_xSe$/CdSe spherical quantum dot-quantum well nanostructure were calculated taking into consideration geometrical confinement, dielectric mismatch and the self-polarization [5]. Wang studied in detail the third-harmonic generation related to intersubband transitions in GaAs/AlGaAs core/shell spherical quantum dots [6]. Asmaa Ibral et al. studied the self-polarization effects on spectra of spherical core/shell nanostructures using perturbation theory and finite difference method [7]. Xie studied the photoionization and third-order susceptibility of a neutral donor in ZnS/InP/ZnSe core/shells spherical quantum dots with Winternitz-Smorodinsky confinement potential [8].

Furthermore, for simplicity, the infinite barrier model was used in several works due to the high band gap of the core material, such us CdS/HgS/CdS and, ZnS/HgS/ZnS dealing to the rise of the so called quantum shell structures. Indeed, the exciton binding energy in infinite inhomogeneous quantum dot has been studied in detail using simple model [9–12]. Also the intersubband optical absorption in the conduction band of quantum shell with and without impurity has been investigated. For example with hydrogenic impurity A. R. Jafari studied the oscillator strengths [13] and the nonlinear optical properties [14] of both finite and infinite confining potentials from ground to the first and second allowed states, he showed that the value of oscillator strengths and the total refractive index (RI) and absorption coefficient (AC) are strongly affected by inner and outer radius of shell. Very recently, Guo et al. showed that the linear and nonlinear and total optical absorption in the spherical dome shell depend strongly on the inner radius, the outer radius and the cut-off angle of the spherical dome shell [15]. The Hydrostatic pressure and electric-field effects on the electronic and the optical properties of an InAs

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spherical layer quantum dot have been studied by Zuhair [16]. Harutyunyan, using the WKB method obtained the analytical expressions of the energy spectrum and wave functions of charge carriers of an infinite inhomogeneous quantum dots [17]. Holovatsky et al. obtained numerically the energy levels and their related wave functions in a CdSe quantum shell using the spherical Bessel functions expansion [18]. In addition the optical properties of quantum shell where also calculated taking into account the effect of external perturbations such as an electric field [19,20] and a magnetic field [21–23].

Since the discovery of the Aharonov-Bohm effect (A-B effect) which is characterized by The oscillation of the ground state with the magnetic field B, several works confirmed experimentally the A-B effect in a number of QD systems, including InP/GaAs QDs [24] and Ge/Si QDs [25] as well as InAs/GaAs quantum rings [26]. The effect of the A-B oscillation on the intersubband optical absorption in a quantum rings have been studied in detail [27]. Moreover, Gu Li-Ying et al. investigated theoretically the A-B effect on the far-infrared spectra in a GaAs/InAs nanoring containing one and two electrons [28]. Bin li et al. showed the importance of an electric field to tune the A-B oscillation in a quantum ring [29]. Climente et al. investigated the AB effect on the optical properties in the three dimensional quantum rings using the effective mass approximation [30,31]. Furthermore, it has been shown that the A-B effect is more pronounced in inverted core shell quantum structures (barrier/well) such as nanoring [27–31] and inhomogeneous quantum dots quantum wells [18,32] than in conventional core shell quantum dots (well/barrier) [33–36].

To the best of our knowledge, the A-B effect on the linear and non linear intersubband optical absorption in spherical quantum shell has not been done until now. For this, using the effective mass approximation and a diagonalization method, the energy levels and the wave functions of a HgS quantum shell are calculated, then the effect of the A-B oscillations on the linear and non linear absorption coefficients is investigated. The choice of HgS material was mainly due to its well known parameters and his weak effective mass value which allow significant establishment of the A-B oscillation at low magnetic field [32].

2. Theory

We consider a spherical core shell quantum dot for CdS/HgS with inner and outer radius a and b respectively. It have been shown that as the HgS layer is enhanced (1 nm) as the electron becomes more confined only in the HgS layer [9] due to the relatively large conduction band offsets of the CdS/HgS quantum dots (1.35 eV) which will justify the use of the infinite barrier potential model for the lowest-lying electron states calculations in our study [11]. As a result, the confinement potential can be expressed as:

$$V(r)=\begin{cases}0 & a\le r\le b\\ \infty & \text{elsewhere}\end{cases} \tag{1}$$

It should be noticed that this infinite barrier potential model have been widely used in the literature for the calculation of electronic and impurity states in quantum shell [9–14,16–23]

The electron Hamiltonian in the presence of a uniform external magnetic field $\vec{B}$ in the z direction is given by:

$$H=\frac{1}{2m_e^*}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2+V(r) \tag{2}$$

where m^* is the electron effective-mass, e is the free electron charge, c is the speed of light in vacuum, $\vec{A}$ is the vector potential of the magnetic field.

Where $\vec{A}=\left[\vec{B}\times\vec{r}\right]/2$, the Hamiltonians becomes:

$$H=-\frac{\hbar^2}{2m_e^*}\Delta+\frac{eB}{2m_e^*c}L_z+\frac{e^2B^2r^2\sin^2(\theta)}{8c^2m_e^*}+V(r) \tag{3}$$

where $L_z=-i\hbar\partial/\partial\varphi$ is the z component of the angular momentum operator.

For the case of zero magnetic fields the wave function read [18]:

$$\psi^0_{n,l,m}=R_{n,l}(r)Y_{l,m}(\theta,\varphi) \tag{4.a}$$

$Y_{l,m}(\theta,\varphi)$ are the spherical harmonics and the normalized radial function is given by [11,12]

$$R_{n,l}(r)=\left(\frac{2}{R^2_{n,l+1}\left(k_{n,l}\right)-\left(\frac{a}{b}\right)^3R^2_{n,l+1}\left(\frac{a}{b}k_{n,l}\right)}\right)^{1/2}\left[j_l\left(k_{n,l}r\right)-\frac{j_l\left(k_{n,l}a\right)}{y_l\left(k_{n,l}b\right)}y_l\left(k_{n,l}r\right)\right] \tag{4.b}$$

where $j_l(r) and y_l(r)$ are the Bessel spherical functions of the first and the second kind respectively, and $k_{n,l}$ are the roots of the following equation

$$j_l\left(k_{n,l}r\right)y_l\left(k_{n,l}b\right)-j_l\left(k_{n,l}a\right)y_l\left(k_{n,l}r\right)=0 \tag{4.c}$$

In the presence of a magnetic the field the above solution Eqs. (4.a) and (4.b) are used as basis of the wave function which can be expressed as:

$$\psi_{n,L,m}=\sum_{n,l}C_{n,l}\psi^0_{n,l,m}=\sum_{n,l}C_{n,l}R_{n,l}(r)Y_{l,m}(\theta,\varphi) \tag{5}$$

where n, L and m are the new quantum numbers of the wave function $\psi_{n,L,m}$ of the quantum shell under a magnetic field. Consequently we can label the eigenstates of electron according to the largest l component of the wave function $\psi^0_{n,l,m}$ [37].

By replacing Eq. (5) into Eq. (2) and using the fact that $\sin^2(\theta)$ can be expressed as a function of the spherical harmonic function $Y_{2,0}$, as follow $\sin^2(\theta)=\frac{2}{3}-\sqrt{\frac{16\pi}{45}}Y_{2,0}$ [38].

We obtain the following matrix Hamiltonian

$$H_{n',l',n,l}=\frac{\hbar^2}{2m^*}k^2_{n,l}\delta_{n,n'}\delta_{l',l}+m\gamma\delta_{n,n'}\delta_{l',l}+\frac{1}{4}\gamma^2\left[\frac{2}{3}\delta_{l',l}-\sqrt{\frac{16\pi}{45}}\left\langle Y_{l,m}(\theta,\varphi)Y_{2,0}(\theta,\varphi)Y^*_{l',m'}(\theta,\varphi)\right\rangle\delta_{m,m'}\right]\int_a^b R_{n,l}R_{n'l'}r^4dr \tag{6.a}$$

where

$$\gamma=\frac{eB\hbar}{2m_e^*c}\text{and}\left\langle Y_{l,m}(\theta,\varphi)Y_{2,0}(\theta,\varphi)Y^*_{l',m'}(\theta,\varphi)\right\rangle=(-1)^m\sqrt{\frac{10(2l+1)(2l'+1)}{4\pi}}\begin{pmatrix}l'\,2\,l\\000\end{pmatrix}\begin{pmatrix}l'&2&l\\-m&0&m\end{pmatrix} \tag{6.b}$$

Using the Clebsh-gordan coefficients proprieties [38], and from Eqs. (6.a) and (6.b), it is clear that the magnetic field couple only the wave functions with $l+2$ states, similar results was found in references [18,33].

Once the energy levels and their corresponding eigenfunctions are obtained, the linear and third-order nonlinear optical absorption coefficients derived from the density matrix approach and perturbation expansion method [39] are given by