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Magnetic Field Effects on Oscillator Strength, Dipole Polarizability and Refractive Index Changes in Spherical Quantum Dot

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Abstract: We have computed the ground and excited state energies and wave functions of a spherical quantum dot with finite potential barrier in the presence of magnetic field. The oscillator strength, the static dipole polarizability and the refractive index changes are investigated as a function of dot radius and magnetic field strength. The results show that the energy state, the oscillator strength, the static dipole polarizability and the refractive index changes are strongly affected by the magnetic field strength and dot size. It is found that while the magnetic field strength increases, the static polarizability decreases strongly.

Keywords: Spherical quantum dot, oscillator strength, static polarizability, magnetic field effect

1. Introduction

In recent years, among low dimensional nanostructures, the understanding of the electronic and optical properties of quantum dots is a subject of scientific investigation from both theoretical and technological points of view. Quantum dots, in which the motion of electron is confined in all space dimensions, have potential applications in microelectronic and optoelectronic devices such as light emitting diodes, high-speed electro optical modulators, solar cells, far infrared photodetectors, laser amplifiers (wavelength ~10μm). Quantum dots (QDs) are known as artificial atoms because of shell structures and discrete energy levels, like real atoms [1]. QDs are excellent models to apply the basic quantum mechanical principles on the optical applications such as optical transitions, oscillator strength and light-matter interactions [2]. Various physical properties of such structures can be controlled by modifying
the dot size, the confining potential, the geometrical shape, electric and magnetic field, the last two are known as external perturbation. Therefore, the electronic structure and binding energy of QDs have been studied by many researchers [3-10]. In these works, the energy spectra of two- and three electron systems confined in in semiconductor QDs with spherically symmetric confinement potential of finite depth were studied by the variational method [3]. Porras-Montenegro et al.[6] calculated the ground state energy and the binding energy of shallow hydrogenic impurities in spherical QDs using a variational procedure within the effective mass approximation. Hu et al.[10] used the variational and plane wave basis method to calculate ground state energy and ground state binding energy in low dimensional nano-structures.

The external perturbation such as application of electric and magnetic field can provide much valuable information about the confined systems and it has become an interesting probe for the study of the physical properties of QDs. Application of external magnetic field to the confined systems introduces an additional confinement potential [11] and modifies the symmetry of the impurity states and the nature of the wave function [12]. This situation dramatically alters the binding energies and optical properties of impurity energy states. Because of this, a number of researchers have been devoted to the study of magnetic field effects on optical properties [13-30] and other physical properties [31-37] employing various methods and different dot shapes. In the studies mentioned above, Ungan et al.[13] investigated theoretically the effects of hydrostatic pressure, temperature, and electric field effects on the optical absorption coefficients and the refractive index changes in quantum well using the compact density-matrix approach and the iterative method. Mandal et. Al [16] analyzed the optical absorption coefficients of impurity doped QD in presence and absence of noise with special emphasis on the roles played by the electric field, magnetic field and dot confinement potential. Rodríguez-Magdaleno et al. [20] used the effective mass
approximation and a Thomas-Fermi-like model to investigate the effects of hydrostatic pressure on the linear and nonlinear optical absorption coefficients of an asymmetric double $\delta$-doped quantum well. Morales et al.[28] calculated the binding energy and impurity polarizability as a function of both electric field and hydrostatic pressure for a shallow-donor impurity in a GaAs-(Ga,Al)As quantum well. They showed that when the impurity electron cloud is farthest from the impurity site the binding energy decreases, and the system is at its maximum deformation leading to the highest value of polarizability. Zhang et al.[37] solved the Dirac equation using the B-spline Galerkin method to calculate the static quadrupole polarizabilities for hydrogen-like ions in the ground state. Zounoubi et al. [38] studied the magnetic field and the barrier height-effects on the binding energy and the 1s-polarizability of a shallow donor confined in a quantum well wire. A detailed theoretical investigation of the magnetic effects on the binding energies, Zeeman transitions and optical absorption coefficients between the ground and higher excited states was reported by our group in a spherical QD with finite and infinite potential barrier [39]. Holovatsky et al.[40] calculated the effect of magnetic field on the oscillator strength in multi-shell QD with three potential wells. Optical properties of a pyramidal QD subjected the external magnetic field were investigated by Niculescu and Bejan [41]. In the presence of the magnetic and electric field, the linear and nonlinear absorption coefficients and the refractive index changes were carried out in the step-like asymmetric quantum well [42]. From the theoretical point of view, the effects of electric field, magnetic field and potential barrier on the optical absorption coefficients were investigated in detail of a doped QD in presence and absence of noise [43]. Zhang et al. [44] calculated the effects of magnetic field on the linear and nonlinear absorption coefficients in a parabolic QD using the compact density matrix approach. In 2018, Zamani et al.[45] studied the effects of applied magnetic field, temperature and dimensions of the structure on the electromagnetically induced transparency of a GaAs quantum ring. Wu
and Cheng [46] calculated theoretically the magnetic dependence of the optical properties of CdSe nanocrystal QDs by using a perturbation method within the effective-mass approximation. Seddik and Zorkani [47] computed the optical absorption coefficients and transition energies associated with transition between the ground state of a hydrogenic donor impurity to the second conduction levels in the presence of a magnetic field, using variational method. In all the studies mentioned above, the authors have reported the magnetic field effects on the optical transitions between low lying energy states of QDs with different size and shapes and they have used the variational method and the trial wave function in their calculations. We know that the spatial confinement, the magnetic confinement and impurity lead to considerable changes on the electronic energy states and the optical properties of QDs. To the best of our knowledge, for the optical transitions between 1s, 2p, 3d and 4f impurity levels, there exists very minimal work concerning the effect of magnetic field on the oscillator strength, the dipole polarizability and the refractive index changes. Therefore, studies in this field are still important for both theoretical and practical applications of QDs.

In this paper, for the ground and excited states with L=1, 2 and 3, we will be investigating the influence of magnetic field on the oscillator strength, the static dipole polarizability and the refractive index changes in the GaAs/Al\textsubscript{x}Ga\textsubscript{1-x}As QD. For a spherical QD, the wave functions and energy states have been calculated by using a modified variational approach based on Quantum Genetic Algorithm (QGA) and Hartree-Fock Roothaan (HFR) method. We have considered the quadratic Zeeman term as a perturbation term. For both the perturbed and unperturbed energy states, the oscillator strengths, the static dipole polarizabilities and the refractive index changes have been investigated as a function of dot radius and magnetic field strength.

2. Theory and definitions
We take into account a system consisting of a GaAs surrounded by Al\textsubscript{x}Ga\textsubscript{1-x}As with a hydrogenic impurity located at QD center. In the effective mass approximation, in the presence of a uniform magnetic field selected in the z-direction, the Hamiltonian of such a system confined by finite potential barrier can be written as follows [12]

\[ H = H^0 + H', \]

where \( H^0 \) is the unperturbed Hamiltonian of system and it is defined as follows, in atomic units (au), in spherical coordinates

\[ H^0 = \frac{-\nabla^2}{2m^*} - \frac{1}{\epsilon_r r} + \frac{1}{2} \gamma L_z + V_C(r), \]

where \( m^* \) and \( \epsilon_r \) are the effective mass of electron and the dielectric constant of material. Here, \( L_z \) is the z component of the angular momentum operator of the electron. The term \( V_C(r) \) is the confinement potential and it has the following form: \( V_C(r) = 0 \) when \( r \leq R \) and \( V_C(r) = V_0 \) when \( r > R \), in which \( R \) is dot radius and \( V_0 \) presents the barrier height.

The term \( H' \) in Eq.(1) is the perturbation Hamiltonian and it is given by

\[ H' = \frac{1}{8} \gamma^2 r^2 \sin^2 \varphi, \]

in which \( \gamma = a_0^* eB / \hbar \) denotes a dimensionless measure of the magnetic field strength, \( a_0^* \) is the effective Bohr radius, and \( \varphi \) is the angle between \( r \) and z axis.

The term \( \gamma L_z \) in Eq.(2) originates from the precession behavior of orbital angular momentum vector \( (L) \) in the magnetic field. This term describes the linear part of the interaction energy between the external magnetic field and the orbital magnetic dipole moment of the electron. The external magnetic field removes the \( m \) degeneracy on impurity energy levels, that is, energy levels are split. The splitting is associated with what is called the angular momentum quantum number \( (l) \) and each level is split into \( 2l+1 \) terms. The term \( \gamma L_z \)
is also called the paramagnetic term and it is sometimes known as linear Zeeman effect. Since the paramagnetic term is proportional to $\gamma$, it causes splitting of energy levels. Similarly the term $H'$ is known as the quadratic term or Quadratic Zeeman effect. The quadratic term is proportional to $\gamma^2$ and it causes shifts at linear Zeeman energy levels. The Hamiltonian $H$ stays difficult to be resolved exactly because it involves two potential: one is the impurity attraction and the other is the magnetic potential. A perturbation method can be used to overcome this difficulty [47]. When $H'$ is compared to $H^0$, it is small and it can be taken into account as the perturbation term in low magnetic field strengths [12].

The Schrödinger equation for the unperturbed Hamiltonian $H^0$ is given by

$$H^0\psi^{(0)}_{nlm}(r) = E^0\psi^{(0)}_{nlm}(r)$$

where $\psi^{(0)}$ is the unperturbed one-electron wave function and $nlm$ are the quantum numbers. For the spherical QD with finite confining potential, the unperturbed wave function is written as follows

$$\psi^{(0)}_{nlm}(r) = \Theta(R - r)\psi^{r<R}_{nlm}(r) + (1 - \Theta(R - r))\psi^{r>R}_{nlm}(r),$$

in which $\Theta(R - r)$ is the Heaviside step function. Here, $r<R$ ($r>R$) shows the situation inside (outside) the well. In HFR approach, the spatial part of the normalized one-electron wave function can be written as linear combination of Slater type orbitals (STOs), $\chi_k$, called basis functions,

$$\psi_p = \sum_{k=1}^{\sigma} c_{pk} \chi_k,$$

where $\sigma$ is the size of STOs and $c_{pk}$ is the expansion coefficients. In the present study, we have employed the unnormalized complex STOs.

The calculation of ionic contribution to the electric field gradient in solids requires the knowledge of accurate values of dipole polarizability. The dipole polarizability of a system
corresponds to a dipole moment induced in the system interaction with an external electric field. The polarizability describes in the lowest order the distortion of the electron cloud in the presence of an external uniform electric field and it is associated with many physical quantities such as the refractive index, the dielectric constant, the ion mobility in the gas, the Van der Waals constant and the long range electron-impurity interaction potential [48]. When a confined system is subjected to a time–independent electric field –static case– in the z-direction, the static dipole polarizability in terms of oscillator strength can be expressed by [37,49]

\[ \alpha_d = \sum_{f>i} \frac{P_{i\rightarrow f}}{(E_f-E_i)^2} \]  

(6)

where \( E_f \) and \( E_i \) shows excited and low impurity energy states. Here, the summation is over all the bound and continuum states. The computation of the static polarizability using sum-over states needs accurate evaluation of wave functions and energies of the system. The accurate evaluation of the integrals over all continuum states is very complex for the present numerical capability [50]. For the 1s polarizability, the transition from one-shell to three shell does not change the polarizability. This is due to the fact that the major contribution to the 1s polarizability comes from 1s\( \rightarrow \)2p transition and is not significantly modified by appearance of new p states in additional shells, owing to the great value of the energy difference between the 1s and 2p states [51]. Therefore, in the present study, this sum has been terminated after two cases including 1s\( \rightarrow \)2p and 1s\( \rightarrow \)3p dipole transitions. The term \( P_{i\rightarrow f} \) in Eq.(6) is oscillator strength. The strength of optical transitions due to interaction of spherical QD with the applied radiation is commonly expressed in terms of a dimensionless quantity called oscillator strength. The oscillator strength is a physical quantity of practical importance in the study of the optical property. It determines the intensity of a specific spectral line in atomic spectrum [52] and it can also offer additional information on the fine structure. The oscillator strength
for transitions from lower state $i$ to higher state $f$ in the spherical QD with finite potential barrier, corresponding to absorption or emission of photons, is given by [49]

$$ P_{i\rightarrow f} = 2\left| \langle M_{i\rightarrow f} \rangle^{R<} + \langle M_{i\rightarrow f} \rangle^{R>} \right|^2 (E_f - E_i). \tag{7} $$

where $\langle M_{i\rightarrow f} \rangle = \left| \psi_f^{(0)} | r \cos \theta \rangle \psi_i^{(0)} \right|$ is the dipole matrix transition element between $i$ and $f$ states, $r$ is the distance between electron and impurity and $\theta$ shows the angle between the position vector and the applied field. The dipole transitions are allowed only between the states satisfying the selection rules $\Delta l = \pm 1$ and $\Delta M = m' - m = 0$ and $\pm 1$.

The linear and the third-order nonlinear optical refractive index changes, which are dependent on position-dependent effective mass, of a spherical nano-system from low state $i$ to allowed excited state $f$ can be expressed as [53-57]

$$ \frac{\Delta n^{(1)}(\omega)}{n_r} = \frac{\rho}{2n_r^2 \varepsilon_0} \left| \langle M_{i\rightarrow f} \rangle^{R<} + \langle M_{i\rightarrow f} \rangle^{R>} \right|^2 \frac{E_f - E_i - \hbar \omega}{(E_f - E_i - \hbar \omega)^2 + (\hbar \Gamma_f)^2}, \tag{8} $$

and

$$ \frac{\Delta n^{(3)}(\omega, I)}{n_r} = \frac{\rho \mu \alpha c}{n_r^2 \varepsilon_0} \left| \langle M_{i\rightarrow f} \rangle^{R<} + \langle M_{i\rightarrow f} \rangle^{R>} \right|^4 \frac{E_f - E_i - \hbar \omega}{[(E_f - E_i - \hbar \omega)^2 + (\hbar \Gamma_f)^2]^2}, \tag{9} $$

where $n_r = \sqrt{\varepsilon_r}$ denotes the static component of refractive index in the semiconductor, $I = 2 \varepsilon_0 n_r c |\tilde{E}|^2$ is the incident optical intensity, $c$ is the speed of light in vacuum, $\tilde{E}$ is the electric field of incident wave, $\mu = 1/\varepsilon_0 c^2$ is the magnetic permeability and $\tau_f = 1/\Gamma_f$ is the relaxation time, respectively. It should be noted that for more realistic calculations, the electron density $\rho$ is calculated from $\rho = \frac{n}{V_{QD}}$, where $n$ is the number of electrons in QD and $V_{QD}$ is the volume of QD [58].

The total refractive index changes are given by
As seen in Eq. (9), the third-order nonlinear refractive index changes \( \Delta n^{(3)}/n_r \) is negative and proportional to the incident optical intensity \( I \). Therefore, as the value \( I \) increases, the total refractive index change \( \Delta n/n_r \) significantly reduced by the nonlinear term.

3. Results and Discussion

In this study, the external magnetic field effects on the oscillator strength, the static dipole polarizability and the refractive index changes have been investigated for the spherical QD, GaAs/Al\(_x\)Ga\(_{1-x}\)As. The atomic units have been used throughout the calculations, where the electron mass \( m_0 = 1 \), the Planck constant \( h = 1 \), and the electronic charge \( e = 1 \). We have used the material parameters of GaAs for the well region and Al\(_x\)Ga\(_{1-x}\)As for the barrier region since their physical parameters are well known, \( x \) is stoichiometric ratio, which is sometimes called Aluminium concentration ratio. The difference between the band gaps of GaAs and Al\(_x\)Ga\(_{1-x}\)As is \( \Delta E_g(x) = (1.155x + 0.37x^2) \text{ eV} \), the effective dielectric constant is \( \varepsilon(x) = (13.18 - 3.12x) \), the effective electron mass is \( m^*(x) = (0.067 + 0.084x)m_0 \), \( m_0 \) is the free-electron mass. We have used 60\% of the band gap difference for the confining potential as suggested in the literature [59]. Using the above given parameters for GaAs\((x=0)\), the effective Rydberg energy is \( R^*_1 \equiv 5.72 \text{ meV} \) and the effective Bohr radius is \( a_1^* \equiv 101\text{\AA} \). The effective electron mass is \( m_{GaAs}^* = 0.067m_0 \) and the effective dielectric constant is \( \varepsilon_{GaAs} = 13.18 \). Also the effective masses of electrons inside GaAs and Al\(_x\)Ga\(_{1-x}\)As are \( m_1^* \) and \( m_2^* \) and the dielectric constants are \( \varepsilon_1 \) and \( \varepsilon_2 \), respectively. The position dependent effective mass and the dielectric constant may be defined as follows [60]:

\[
m^*(x) = \begin{cases} 1, & r < R \\ \frac{m_2^*}{m_1^*}, & r > R \end{cases} \quad \text{and} \quad \varepsilon(x) = \begin{cases} 1, & r < R \\ \frac{\varepsilon_2}{\varepsilon_1}, & r > R \end{cases}
\] (11)
On the other hand, the unperturbed energy has been calculated, we have considered the unperturbed energy as the energy inside well plus the energy outside well, that is \( E^0 = E^<R + E^>R \). The calculation of these energy integrals are given in Ref. [61]. Also, in calculations of the refractive index, we used the parameters \( n_r = 3.2 \) and \( \tau = 0.4ps \). For a given value of the magnetic field \( B \), the \( \gamma \) value may be very different from one semiconductor to another since it depends on both the effective mass and the electrical permeability values. For example, the value of \( \gamma = 1 \) corresponds to the magnetic field \( B = 6.62T \).

It is preferred to use the Slater type orbitals (STOs) in the quantum mechanical analysis of the electronic structure of QD since they show correct behaviour of the electronic wave functions. Therefore, we have chosen a linear combination of s (or p,d,f) STOs, which are of different screening parameters for a s (or p,d,f) type atomic orbital. In order to maintain the orthogonality of orbital, the same set of screening parameters has been used for all one-electron spatial orbital with the same angular momentum and the orbital set of each individual has been orthonormalized using the Gramm-Schmidt procedure. In order to determine the expansion coefficients and the screening parameters of the wave function minimizing the total energy, we have employed a modified variational approach which is a combination of QGA procedure and HFR method, whose details are given in Refs.[62,63], and we have used seven basis functions to calculate the energy expectation value.

In Fig.1, we have plotted the 2p-energy state at \( x = 0.3 \): (a) as a function of dot radius for two different values of \( \gamma \) and (b) as a function of \( \gamma \) for three different values of \( R \). In (a), as the dot radius increases, the energy decreases. And when the dot radius is large enough, at the fixed \( \gamma \), the energy goes to a constant value. As seen in (a), when \( \gamma \neq 0 \), 2p-energy state splits symmetrically according to the state \( m = 0 \) due to the paramagnetic term. For the \( |m| \) values,
the splitting is increasing as the $\gamma$ increases. The results are similar to the results obtained
exact diagonalization and variational method [11,12].

In (b), as the $\gamma$ increases, the energy increases linearly, as expected. It is seen that this
linearity does not change as the dot radius increases.

In order to see how the magnetic confinement affects the oscillator strength, in Fig.2, we
show the oscillator strength for the 1s-2p, 2p-3d and 3d-4f optical transitions between the
unperturbed states as a function of dot radius at four different values of the $\gamma = 0, 0.2, 0.5$
and 2. As seen from the curves, the oscillator strength shows similar behaviors. As the dot
radius increases, first the oscillator strength is climbing rapidly and then reaches maximum
value at a certain dot radius. Afterwards it is decreasing monotonically again and then it goes
to a constant value in very large dot radii. The influence of the magnetic field which is
originated from the paramagnetic term appears clearly on the oscillator strength. When $\gamma \neq
0$, both the peak position of the oscillator strength shifts towards larger dot radii and the
oscillator strength increases as the magnetic field increases. In (a), 1s $\rightarrow$ 2p transition, the s-
level is unaffected from the magnetic field, but 2p level is affected. Therefore, the magnetic
field removes the $m$ degeneracy on 2p level and it is split into three sublevels ($m = 0, \pm 1$)
due to the paramagnetic term (or Zeeman effect). In the case of $m = +1$, since the positive
contribution coming from the paramagnetic term shifts upwards the Zeeman energy level, the
energy interval between 1s and 2p levels increases in the case of $\Delta M = +1$, see [39]. Thus,
peak positions of the oscillator strengths move towards right (blue shift) with the increase of
the transition energy. In (b) and (c), in the cases of $m' - m =2-1$ and 3-2, the oscillator
strengths exhibit the similar behaviors. As seen in (b) and (c), since the energy contribution
coming from paramagnetic term is larger, the peak positions of the oscillator strength shift
towards larger dot radii.
In Fig. 3, we have shown the oscillator strength for $1s \rightarrow 2p$ and $2p \rightarrow 3d$ transitions as a function of $\gamma$ for three different values of dot radius $R=1$, $3$ and $4$. As seen from oscillator curves, in small dot radius $R=1$, the oscillator strength is relatively insensitive to the increase of $\gamma$. That is, as the value of $\gamma$ increases, the variation of oscillator strength remains almost the same at the beginning and at the end of the curve. However, in large dot radii, for example $R=3$ and $4$, the oscillator strength increases with the increase of the magnetic field. The oscillator strength of the transition between unperturbed levels (solid line) increases linearly with the increase of $\gamma$. Whereas, in the perturbed levels, the oscillator strength (dashed line) increases monotonically. This phenomenon stems from the diamagnetic term considered as perturbation. This term behaves like power law proportional to $r^2$ and $B^2$ in large dot radii and magnetic field strengths. As seen in (b), the oscillator strength increases in the transitions between higher levels. This is because the wave functions of the states with bigger $l$ have a larger spatial extent resulting in larger diamagnetic interaction energies.

For the optical transitions between the unperturbed levels in the case of $\Delta M = +1$, the variation of $1s$, $2p$ and $3d$ static dipole polarizability is shown in Fig. 4 as a function of dot radius for four different values of the magnetic field strength. The dominant contribution to the $1s$ polarizability comes from the $1s \rightarrow 2p$ transition because of the energy difference between the $1s$ and $2p$ levels. The $1s$ polarizability is not significantly modified by the appearance of new $p$ states in additional shells [51]. In $x=0.3$ and $\gamma = 0$, for the $1s$ polarizability, in very large dot radii, for example $R=20$, in which the values of energy, oscillator strength and polarizability in the QD approach the corresponding the values of hydrogen atom, we have calculated $0.41970$ au and $0.11015$ au for $1s \rightarrow 2p$ and $1s \rightarrow 3p$ oscillator strengths and $2.98294$ au and $0.54065$ au for $1s \rightarrow 2p$ and $1s \rightarrow 3p$ static polarizability values. The literature values are $0.4160$ au and $0.07910$ au for $1s \rightarrow 2p$ and $1s \rightarrow 3p$ oscillator strengths and the static dipole polarizability values are $2.96283$ au and
0.40067 au for $1s\rightarrow2p$ and $1s\rightarrow3p$ static polarizability values of hydrogen atom [65]. Our results are in good agreement with literature results. Similarly, for the $2p$ and $3d$ polarizabilities, the major contribution comes from the $2p\rightarrow3d$ and $3d\rightarrow4f$ transitions. It is seen that both the spatial confinement and the magnetic confinement have a great influence on the polarizability. While both the dot radius decreases and the magnetic field increases, the polarizability decreases. Both positive effects tend to decrease the spatial extension of the wave function and so the polarizability of the system changes. The polarizability curves exhibit the similar behaviors in all transitions. As will be seen in (a), in larger dot radii $R>15$, $1s$ polarizability reaches a saturation value and then it does not change anymore and remains constant. As the dot radius decreases, after a maximum value, the polarizability starts to decrease and continues to decline until reaching to a certain minimum point and then it increases rapidly again when the dot radius $R$ becomes very small (or in the strong confinement region). The reason of this behavior can be explained as follows: as the dot radius decreases, the bound electron wave function is very localized due to the confining potential barrier and so the polarizability decreases. If the dot radius continues further decreasing in the strong confinement region, the wave function escapes out of the dot toward the material barrier, and the polarizability of the system starts to increase rapidly again and becomes maximum. On the other hand, in the strong confinement region, $R<1$, since the electronic orbital is very localized, the charge distribution becomes less sensitive to the magnetic field, and so the magnetic confinement is insensitive on the polarizability in this region. In this region, the effect of the spatial confinement is more dominant than the magnetic confinement. Therefore, the situation of polarizability is determined by spatial confinement. As a consequence, in the strong spatial confinement region, it needs sufficiently strong magnetic field to overcome the strong spatial confinement. In the intermediate confinement region ($1<R<3$), in which the effect of spatial confinement on electron mixes
with the effect of the magnetic confinement, the polarizability begins to become sensitive to the magnetic field. As for the weak spatial confinement region (R$\geq$3), the magnetic confinement on electron prevails over the spatial confinement, and the polarizability is more sensitive to the magnetic field. As seen in polarizability curves, a very important feature is that as the magnetic field increases, the polarizability decreases in the weak confinement regions. On the other hand, in (b) and (c), the similar behaviors have been obtained for 2p and 3d static polarizability. Since 3d and 4f orbitals are more external orbitals according to 1s and 2p, the polarizability values are larger and the peak positions of polarizability shift towards large dot radii, as expected. For 1s polarizability, a similar behaviour has been reported by [38] for the quantum well wire. For higher levels, we were not able to compare to our results since there are no theoretical results in literature.

In Fig.5, for transitions in the case of $\Delta M = +1$, we have plotted the variation of polarizability as a function of magnetic field for the perturbed (dashed line) and unperturbed (solid line) 1s, 2p and 3d states at four different values of dot radius R=1,3,4 and 5. It is clearly seen in polarizability curves that as the magnetic field increases, the polarizability decreases with increasing dot radius, except for the case R=1. In the strong confinement region, the polarizability is totally insensitive to the increase of magnetic field, like oscillator strength. Since the electronic orbital is very compressed (localized) in the strong spatial confinement region, the effect of the magnetic field on the charge distribution is very weak. Therefore, the polarizability does not change as the magnetic field increases. In large dot radii, as the magnetic field increases, the polarizability decreases due to the charge distribution shrinking. The electron is pushed inward and approaches to impurity due to the confinement effect of magnetic field, and so the polarizability becomes significantly reduced with the increase of magnetic field. As a result, it can be said that the polarizability follows the binding energy variation closely. In large dot radii, the electron cloud is pushed by the
magnetic field towards the impurity, and so the binding energy increases. It is true on the contrary. That is, as the electron cloud moves away from the impurity, the binding energy decreases and so the polarizability increases, as in Fig.4. The computed polarizability values have reasonable magnitudes and correctly reflect the effect of the magnetic field, which confines the electron more and decreases the polarizability. On the other hand, as seen in curves, at fixed dot radius, the polarizability of the perturbed level decreases further as the magnetic field increase, especially in large dot radii. This is because the diamagnetic term behaves like a power law in large magnetic field strength as it is proportional to $B^2$. The increase in the magnetic field causes more shrinkage of the wave function, and so the polarization is further reduced.

The refractive index is an important parameter in investigation of optical properties. In order to investigate the influence of magnetic field on the refractive index changes, in Fig. 6, we have plotted the refractive index changes as a function of photon energy $h\nu$ for the optical transitions between the unperturbed 1s, 2p, 3d and 4f levels in the case of $\Delta M = +1$ and 5. As the photon energy increases, the refractive index change increases constantly until reaching maximum value, which happened in the normal dispersion, defined $dn/d\omega > 0$, and then the refractive index curve falls to a minimum value with increasing photon energy. After a minimum, it inclines monotonically again with the increase of photon energy. As the photon energy approaches the threshold energy, the sign of normal dispersion changes and it becomes negative. The region between extreme values is more commonly named the anomalous dispersion, which is defined by $dn/d\omega < 0$. It is well known that pulses of light can achieve speeds greater than $c$ in regions of anomalous dispersion, and inside an absorption line, the dispersion is anomalous, resulting in a group velocity faster than $c$, the vacuum speed of light [65]. Regions of anomalous dispersion always occur around absorption frequencies, because there is a direct connection between the refractive index and the absorption of a material. The
anomalous dispersion happens in areas of rapid spectral variation with respect to the refractive index and it allows for a negative contribution to the group velocity. The anomalous dispersion is found in the resonance frequency of the spherical QD. Since photon is very strongly absorbed, this region is known as an absorption band. As seen in the refractive index curves, the total refractive index change is significantly reduced by the nonlinear contribution because the sign of the nonlinear term is negative. Also, the contributions of both the linear and the third-order nonlinear refractive index changes should be considered especially for those operating under high incident optical intensity $I$. In (a), at a fixed dot radius and magnetic field value, the peak position of the refractive index in transitions between the bigger $l$ levels moves towards higher energy because of the increase of energy difference. In (b), the effect of magnetic field is clearly seen on the refractive index curves. When compared (a) to (b), as the external magnetic field increases, the peak positions of all transitions shift towards the higher energy (blue shift) due to the paramagnetic term. The energy level is split into more sublevels due to the paramagnetic term in the presence of magnetic field. While the magnetic field strength $\gamma$ increases, the sublevels move away from each other, and the transition energy between sublevels increases. Thus, the transition energy shifts towards higher energies (blue shift). For example, while $\gamma = 1$, the peak position energies of the linear refractive index change are 2.95 au, 3.92 au and 3.59 au for the transitions $1s \rightarrow 2p$, $2p \rightarrow 3d$ and $3d \rightarrow 4f$ and their peak heights are 0.2238, 0.3968 and 0.5071. While $\gamma = 5$, these values are 4.92 au, 5.15 au and 5.57 au for the transitions $1s \rightarrow 2p$, $2p \rightarrow 3d$ and $3d \rightarrow 4f$ and their peak heights are 0.2404, 0.4205 and 0.5394. It can be said that while the peak position is directly linked to the value $\gamma$, the peak height depends on the matrix element. For the $1s$-$2p$ transition, the similar results have been reported by [66].

Fig.7 shows the linear, nonlinear and total refractive index changes as a function of photon energy for transitions between the perturbed $1s$, $2p$ and $3d$ levels in the case of $\Delta M = +1$. As
seen from figure curves, the refractive index depends strongly on dot size. It is readily seen that, at a fixed value of $\gamma$, the refractive index changes in small dot radius are much stronger than large dot radius. This is because, the refractive index change depends on the QD volume as $1/V_{QD}$, and so the magnitude of the refractive index change increases as the dot radius decreases. In addition, the peak positions of the refractive index shift towards higher energy (blue shift) as dot radius decreases. The reason is that the energy difference between levels is greater in small dot radii. On the other hand, it is seen that the nonlinear term increases faster in large dot radii. Similar behaviors are seen in the transitions 2p-3d. However, it is worth to note that the amplitudes of the transitions between higher levels are greater than those of lower levels. The results are similar to the results obtained by Zounoubi et al.[38] for the GaAs quantum well wire.

**Conclusion**

In this paper, in the presence of an external magnetic field, we have calculated the unperturbed ground and several excited state energies and the wave functions of the spherical QD with finite potential barrier by using QGA procedure and HFR method. We have investigated in detail the magnetic field effect on the oscillator strength, the static dipole polarizability and the refractive index change for the fundamental and higher transitions. It is observed that, in strong confinement region $R \leq 1$, while the effect of the magnetic field on the QD is very weak, the effect of spatial confinement is very strong since the charge distribution is very strongly localized inside the QD. Thus, in this region, the effect of the magnetic field is insensitive to the oscillator strength, polarizability and refractive index. In the dot region $1 < R < 4$, the magnetic confinement and the spatial confinement effects are inside a competition with increasing dot radius. In large dot radii, in the weak confinement region, $R \geq 4$, the situation is exactly opposite and the magnetic field plays a more important role on the oscillator strength, static polarizability and refractive index change. In large dot radii, it is
found that the static polarizability decreases as the magnetic field increases. The increase of magnetic field in large dot radii shrinks the electron wave function and decrease the cyclotron radius for the electron. Thus, the magnetic confinement compels the electron to move ‘closer’ to the impurity and so the static polarizability decreases. In large magnetic field and dot radius, since the diamagnetic term behaves like a power law due to $B^2$ and $R^2$, this term supplies major contribution to energy levels and so the peak positions of the refractive index changes shift towards higher energy. Theoretical investigation of the magnetic effects on the physical parameters such as energy state, oscillator strength, static dipole polarizability and refractive index change of spherical QD will lead to a better understanding of the properties of low dimensional structures. Such theoretical studies may have profound consequences about practical applications of the electro-optical devices, and the results of this study will contribute to the research on related subjects.

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References


Fig. 1 Variation of 2p-energy state: (a) as a function of dot radius and (b) as a function of magnetic field strength $\gamma$. 
Fig. 2 Variation of oscillator strength for 1s-2p, 2p-3d and 3d-4f dipole transitions between the unperturbed levels as a function of dot radius for four different values of magnetic field: $\gamma = 0, 0.2, 0.5$ and 2. $\gamma = 0.2$ corresponds to a magnetic field strength of 1.324 T.
Fig. 3 Variation of oscillator strength in 1s-2p and 2p-3d dipole transitions in the case of $\Delta M = +1$ as a function of magnetic field at $x=0.3$ for three different values of dot radius: $R = 1, 3$ and 4 (dashed line for perturbed states and solid line for unperturbed states).
Fig. 4 Variation of 1s, 2p and 3d static dipole polarizability as a function of dot radius at x=0.4 for four different values of the magnetic field strength γ: 0.2, 0.5, 1 and 2.
Fig. 5 Variation of 1s, 2p and 3d static dipole polarizability as a function of the magnetic field strength $\gamma$ at $x=0.3$ for four different values of dot radius: $R = 1, 3, 4$ and 5 (dashed line for perturbed states and solid line for unperturbed states).
Fig. 6 Refractive index changes for the optical transitions between the unperturbed 1s, 2p, 3d and 4f levels as a function of photon energy at $x=0.4$ and $I=30\times10^6$ W/m$^2$ for two different values of magnetic field strength: $\gamma=1$ and 5.
Fig. 7 Refractive index changes in transitions between the perturbed levels as a function of photon energy for three different values of the dot radius at $\gamma = 2$, $x = 0.4$ and $I = 3 \times 10^6 \text{W/m}^2$. 
Graphical abstract
Highlights

The unperturbed wave functions and energy states of spherical quantum dot are obtained from QGA and HFR method.

Magnetic Field Effects on Oscillator Strength and Dipole Polarizability are investigated.

Effects of Magnetic Field on Refractive Index Changes are also studied.