Journal of Basic and Applied Engineering Research
p-ISSN: 2350-0077; e-ISSN: 2350-0255; Volume 5, Issue 4; April-June, 2018, pp. 311-315

http://www.krishisanskriti.org/Publication.html

To Study the Relativistic Effect under the Magnetic Field on the Linear and Nonlinear Optical Absorption Coefficients and Refractive Index Changes in 3-D GaAs Quantum Dot.

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Abstract—*In this study, the linear and nonlinear optical absorption coefficient and refractive index of inter sublevel transitions have been calculated for 2-electron quantum dot with spherical harmonic oscillator type potential. The electron Eigen energies and the corresponding wave functions have been determined analytically and optical properties have been determined using dipole approximation within the effective mass approximation. We have investigated the effects of the relativistic and non-relativistic corrections to kinetic energy, Darwin term and spin-orbit interaction for the zero-dimensional structure in the presence of weak magnetic field to the energy Eigen values and wave functions for GaAs. The effect of confinement potential on linear and nonlinear optical absorption coefficients and refractive index has been studied. It is found that the size of the depth of the confinement have a profound effect on the linear and nonlinear absorption coefficients, when relativistic corrections are taken in account.*

Keywords*: Quantum dot, Optical properties, Relativistic corrections, Confinement potential.*

1. INTRODUCTION

In the past two decades, there has been a speedy development in the field of nanoscience and nanotechnology. Hence the study of low-dimensional semiconductor structures also known as artificial atoms or nanostructures becomes essential. These nanostructures including quantum wells, quantum wires, and quantum dots (QDs), differ in size from the macroscopic structures and hence possess some interesting and unique properties [1,2]. Because of these some unique properties, scientists have shown much interest in the nanostructures, as they offer a wide area of research for them [3]. Charge carriers in nanostructures are confined in one, two, and three dimensions. Out of these three classes, the class of zero-dimensional structures also called as quantum dots, in which charge carriers are confined in all the three dimensions, is the most intensively studied class of semiconductor structures. This quantum confinement of charge carriers leads to some unique changes such as formation of discrete energy levels, increase in the density of states at some specific energies and the extreme change of optical absorption spectra [4].

Linear and nonlinear optical properties such as optical absorption and refractive index changes have some wide potential applications in optoelectronic and photonic devices such as in far-infrared laser amplifiers, photo detectors, and high speed electro-optical modulators, hence these properties of quantum dots have been widely studied under some external factors including spin–orbit interaction, electron–phonon interaction, magnetic field, electric field, temperature, impurity and pressure [5-12].

In the present work, we have studied the effect of relativistic corrections on the optical properties in the GaAs quantum dots, as the study of electronic and optical properties of quantum dots has been considered as an important challenge in the physics science. The energy levels and the modified wave functions for both the ground (1s) and first excited (1p) states in the presence of weak magnetic field and relativistic effects in terms of perturbations were computed analytically and optical properties have been determined using the dipole approximation within the effective mass approximation. The effect of relativistic corrections on the optical parameters have been calculated as a function confinement potential. To the best of our knowledge, no investigations have been done so far to understand the dependence of linear and nonlinear optical properties such as optical absorption and refractive index on confinement potential with relativistic corrections to the kinetic energy, Darwin term and spin-orbit interactions.

The paper is organized as follows. In Section 2 we first give a theoretical background on the problem considered. The main idea of our approach is then summarized in the same section. In the same section the Relativistic corrections to the energy states are described. Section 3 describes the various optical properties mathematically. Section 4 is dedicated to the results of the calculations and their probable physical reasons are discussed and finally, the paper ends with a brief summary and concluding remarks.

2. THEORY AND MODEL

Energy Levels and Wave Functions

Here we are considering a two-electron spherical Quantum dot in the presence of magnetic field under the confinement spherical harmonic oscillator potential for GaAs quantum dot is modelled as:

$$V(r_i) = -V_0 e^{\frac{-r_i^2}{2R_P^2}} \quad (1)$$

Where $V(r_i)$is the confinement potential of the quantum dot,r_i is the position coordinate of the i^{th} particle, V_0 is the depth potential and R_P give the measure of Range of confinement potential which represents the size of quantum dot and P represents the hydrostatic pressure.

Under the approximation $r_i \ll R$,The unperturbed Hamiltonian H_0 reduces to

$$H_0 = -\frac{\hbar^2}{2m_P^*}\sum_{i=1}^{N}\nabla_{r_i}^2 + \gamma^2\sum_{i}^{N} r_i^{\,2} \quad (2)$$

The non-relativistic Hamiltonian of a system of 2 electrons in a spherical quantum dot under the electric and magnetic fields (2) can be written as:

$$H_T = H_0 + H_{pot}{}' + H'_{M1} + H'_{M2} + H'_{M3} \quad (3)$$

$$\text{Where,} H'_{pot} = \sum_{i=1}^{N} -\frac{e^2}{\varepsilon_P r_i} - NV_0 \quad (4)$$

Here 1st two terms i.e.$H_0 + H_{pot}{}'$ represent the contribution of hydrogenic Impurity

The third term represents the energy due to the interaction between particles orbital magnetic dipole moment $\left(\frac{qL}{2cm_p}\right)$and magnetic field B.

$$H'_{M1} = -\frac{qBL\cos\cos\varphi}{2m_P^* c} \quad (5)$$

The fourth term gives ratio of the paramagnetic and diamagnetic contribution which is very small and thus can be ignored.

And, shift due to Magnetic energy correction is given by the Paschen Back effect as

$$H'_{M3} = <\Psi_{nlm}\left|\frac{eBL_{iZ}}{2m_P^* c}\right|\Psi_{nlm}> = \Delta E_B = B\mu_B \quad (6)$$

The Schrodinger equation with spherical symmetric harmonic oscillator potential (4) is exactly solvable with the following Energy spectrum:

$$E_{n_i l_i} = \sum_{i=1}^{N}(2n_i + l_i + \frac{3}{2})\hbar\omega \quad (7)$$

where$n_i l_i = 0, \pm 1, \pm 2, \ldots \ldots$

The Eigen values E_T for the Hamiltonian (5) is given by the Schrodinger equation:

$$H_T\Psi_{nlm} = E_T\Psi_{nlm} \quad (8)$$

For any arbitrary state, the complete wave function, ψ(r, θ, ϕ), can be written as

$$\Psi(r,\theta,\varphi) = \sum_{nl} N_{nl} R_{nl}(r) Y_l^m(\theta,\varphi) \quad (9)$$

Where the radial wave function $R_{nl}(r)$ is the solution of the equation

$$\left(\frac{d^2}{dr^2} + 2r\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)R_{nl}(r) + \frac{8\pi^2 m}{h^2}[E_{nl} - V(r)]R_{nl}(r) = 0$$

Reducing radial equation to the simple form using the transformation

$$\left[-\frac{\hbar^2}{2m_P^*}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2m_P^* r^2} + \frac{V_0}{2R_P{}^2}r^2 - E_{nl}(r)\right]u_{nl}(r) = 0 \quad (10)$$

The general solution of this radial equation is

$$R_{nl}(r) = N_{nl} r^l \exp\left(-\frac{\eta r^2}{2}\right) L_{\frac{n-l}{2}}^{l+0.5}(\eta r^2) \quad (11)$$

Where $\eta^2 = \frac{2m_P^* V_0}{2R^2\hbar^2}$ and $L_b^a(\eta r^2)$ is the generalized Laguerre polynomial.

Here, the normalization constant is defined as

$$N_{nl} = \left[\sqrt{\frac{2^{n+l+2}\eta^{l+1.5}}{\sqrt{\pi}}}\right]\sqrt{\frac{\left(\frac{n-l}{2}\right)!\ \left(\frac{n+l}{2}\right)!}{(n+l+1)!}} \quad (12)$$

Where l= n, n-2, …..$l_{min.}$ andl_{min}= 1 if l is odd and =0 if l is even.

The complicated nature of the recursion relations appeared in solving the complex integral for two interacting electrons confined in three-dimensional dot geometry is given below

$$<\varphi_{nlm}\left|\frac{1}{r_{ij}}\right|\varphi_{nlm}> = \sum_{i\neq j}\sum_{l}\sum_{m}\int_0^\infty |R(r_i)|_{nl}^2 r_i^2\,dr\int_0^\infty |R(r_i)|_{n_1 l_1}^2 r_j^2\,dr\int |Y_l^m(\Theta_1\Phi_1)|^2\,d\Omega_1\int |Y_l^m(\Theta_2\Phi_2)|^2\,d\Omega_2\; Y_l^{*m}(\Theta_1\Phi_1)Y_l^m(\Theta_1\Phi_1) \quad (13)$$

Relativistic corrections:

Energy shift due to Spin-Orbit coupling is given as:

$$\Delta\ \Delta E_{so} = \frac{e^2\hbar^2}{4\mathcal{E}_P m_P^{*2} c^2}\left\{j(j+1) - l(l+1) - \frac{3}{4}\right\} < \Psi_{nl_jm_j}| \sum \frac{1}{r_i^3} |\Psi_{nl_jm_j} > \quad (14)$$

Energy shift due to relativistic correction to Kinetic energy is given as:

$$\Delta E_k = < \Psi_{nlm_lm_s}|H_K|\Psi_{nlm_lm_s} > = -\frac{1}{2m_P^* c^2}\{E_{nl}^2 + \sum_{i=1}^{N} \gamma^4 < r_i^4 >_{nl} + \sum_{i=1}^{N} \frac{2e^2\gamma^2}{\mathcal{E}_P} < r_i^1 >_{nl} + \sum \frac{e^4}{\mathcal{E}_P^2} < \frac{1}{r_i^4} >_{nl} - \sum \frac{2e^2}{\mathcal{E}_P} < r_i >_{nl} E_n - \sum 2\gamma^2 E_n < r_i^2 >_{nl} \quad (15)$$

Energy correction due to Darwin term is given as:

$$\Delta E_D = \frac{\pi e^2\hbar^2}{2m_P^{*2} c^2 \mathcal{E}_P} < \Psi_{nlm}|\delta(r_i)|\Psi_{nlm} > \quad (16)$$

Optical Properties:

The optical absorption coefficient is given by: $\alpha^1(w) + \alpha^3(w, I)$

Where

$$\alpha^1(w) = w\sqrt{\frac{\mu}{\epsilon_r}} \frac{N_c T_{if} |M_{if}|^2}{\hbar((w_{if}-w)^2 + T_{if}^2)} \quad (17)$$

and

$$\alpha^3(w, I) = -w\sqrt{\frac{\mu}{\epsilon_r}} \frac{4N_c T_{if}|M_{if}|^2}{2\varepsilon_0 n_r c\hbar^3\left((w_{if}-w)^2 + T_{if}^2\right)} \left[\frac{|M_{if}|^2}{(w_{if}-w)^2 + T_{if}^2} + \frac{(M_{ff}-M_{ii})^2 (3w_{fi}^2 - 4w_{fi}w)^2 (w_{fi}^2 - T_{if}^2)}{4(w_{fi}^2 + T_{if}^2)((w_{fi} - w)^2 + T_{if}^2)} \quad (18)$$

are the linear and the third-order nonlinear optical absorption coefficients, respectively.

Similarly, the linear and the third-order nonlinear refractive index changes are obtained by:

$$\frac{\Delta n_r^1(w)}{n_r} = \frac{N_c |M_{if}|^2 (w_{if}-w)}{2n_r^2 \varepsilon_0 \hbar((w_{if}-w)^2 + T_{if}^2)} \quad (19)$$

$$\frac{\Delta n_r^3(w,I)}{n_r} = -\frac{N_c I \mu_c |M_{if}|^2 (w_{if}-w)}{2\varepsilon_0 n_r^3 \hbar^3\left((w_{if}-w)^2 + T_{if}^2\right)} \left[\frac{|M_{if}|^2}{(w_{if}-w)^2 + T_{if}^2} + \frac{2T_{if}(M_{ff}-M_{ii})^1}{\left((w_{fi} - w)^2 + T_{if}^2\right)}\left((w_{if}-w)\left(w_{fi}(w_{if}-w) + T_{if}^2\right) - T_{if}^2(2w_{if}-w)\right)\right)] \quad (20)$$

Therefore total refractive index is equivalent to:-

$$\frac{\Delta n_r\ (w, I)}{n_r} = \frac{\Delta n_r^1(w)}{n_r} + \frac{\Delta n_r^3(w, I)}{n_r} \quad (21)$$

3. RESULTS AND DISCUSSION

Here, optical properties such as linear and nonlinear optical absorption coefficients and refractive index of a spherical quantum dot has been studied as a function of confinement potential using effective atomic units (a.u.) for calculations. All the figures have been plotted using both with and without Relativistic effect. Our results are summarized in Figures1 and Figure2. For GaAs, material parameters that have been used are m (0) =1 and Ɛ (0) = 12.9 and all the graphs have been plotted for different potentials such are: V01=136.234 meV, V02=244.110 meV and V03=379.863 meV.

Figure 1(a) and (b) illustrates the linear and nonlinear absorption spectrum in a spherical quantum dot as a function of the incident photon energy in the range of 50meV for two different barrier heights. The effect of confinement is observed clearly on the barrier height. It can be also be seen that the position of the absorption peak shift towards the region of higher energies i.e. corresponds towards the region of blue shift, with the increase in barrier heights. The reason behind this shift is that the energy difference between the 1S and 1P states which is kept increasing with increase in barrier height. It can also be also seen from the figure that higher the barrier height, the sharper is the absorption peak and the absorption peak intensity also will be bigger. This is due to the overlapping of the wave functions which kept increasing with increase in confinement. i.e. V0. Also it can be observed that the relativistic corrections especially the spin-orbit interaction term makes the peaks steeper as well as little higher in energy.

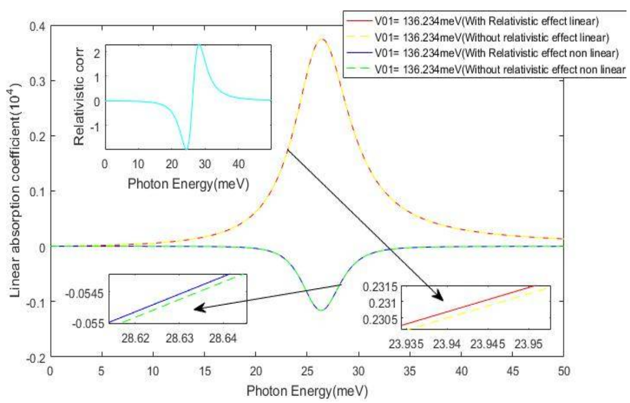

Figure 1(a)

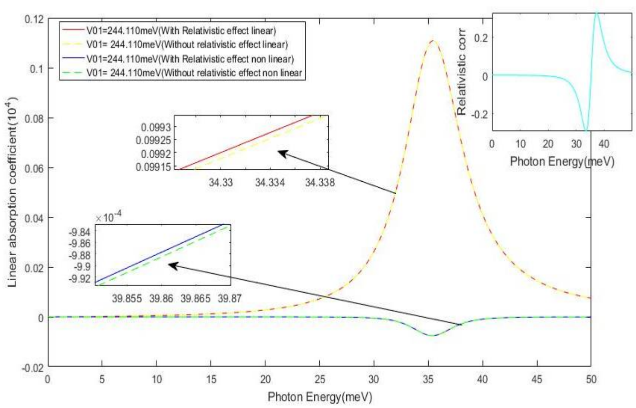

Figure 1(b)

Figure 1(a) and (b): The linear$\alpha^1(w)$, the third-order nonlinear $\alpha^3(w, I)$optical absorption coefficients as a function of the incident photon energy for different values of the barrier height

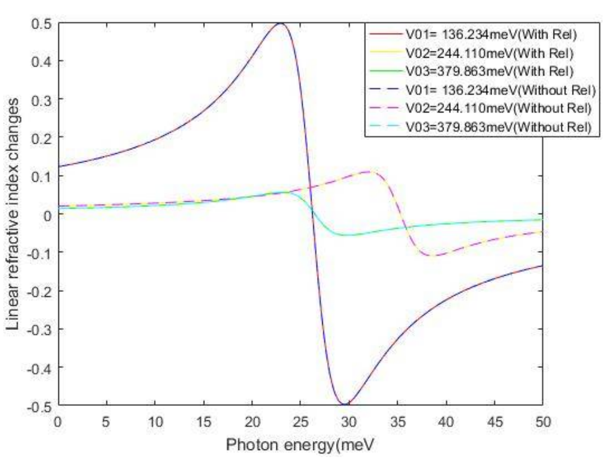

Figure 2(a)

Figure 2(a).The linear, the third-order nonlinear and the total changes in the refractive index as a function of the incident photon energy for three different values of the barrier heights

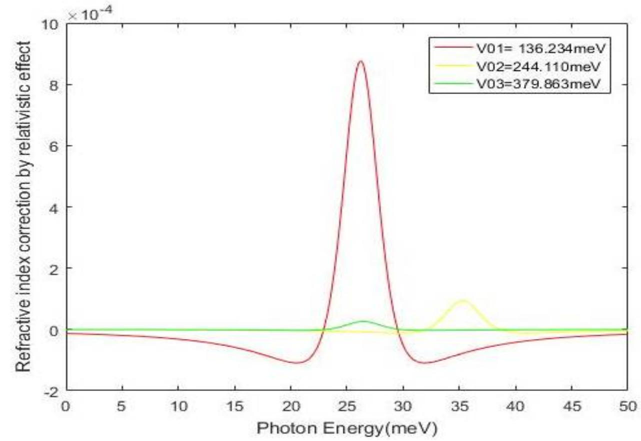

Figure 2(b)

Figure 2(b).Relativistic effect inlinear, the third-order nonlinear and the total changes in the refractive index as a function of the incident photon energy for three different values of the barrier heights.

Figure 2(a) shows the results of the study involving the linear, nonlinear as well as total refractive index in a spherical quantum dot as a function of the incident photon for three different barrier heights. When there is an appropriate relative change in the refractive index, the blue shift is found in energy range, with an increase in the barrier height. With further increase in the barrier height, the change in linear, nonlinear and total refractive index found to be diminished. This happens because of the increase in the energy spacing between the subsequent discrete energy levels as a result of increase in barrier height. Figure 2(b) shows the effect of relativistic correction. As it can be clearly seen from the figure that the peaks are now sharper as well as higher in energy due to the spin-orbit interaction term in the relativistic correction.

4. CONCLUSION

In conclusion, we have calculated the discrete energy spectra for two electrons in a two-dimensional harmonic oscillator that serves as a simple but suitable model for quantum dots on semiconductor interfaces. We have investigated analytically the properties of a quantum dot as a function of confinement potential using dipole approximation within the effective mass approximation under the effect of weak magnetic field, by imposing the relativistic corrections of Pauli's spin– orbit (SO) coupling, Darwin's correction, and mass-velocity (MV) interaction. Our results show that we can obtain a blue shift by simply changing the barrier height, for the inter sub-band transitions in QDs. Applying a relativistic effect to QDs, we can get a significant change in the position and height value of the optical absorption coefficients and refractive index. Our results have a great influence on the experimental studies, and have a great impact on improvement of optical devices such as infrared laser amplifiers, photodetectors, and high-speed electro-optical modulators.

5. ACKNOWLEDGMENT

One of the authors (SD) is thankful to Delhi Technological University, Delhi, India for the financial support. The authors would also like to express their heartfelt gratitude to Prof. Manmohan and Dr. Arun Goyal, University of Delhi for their encouragement and fruitful discussions towards the successful completion of the work.

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