OPTICAL ABSORPTION IN PYRAMID-SHAPED QUANTUM DOTS UNDER APPLIED ELECTRIC AND MAGNETIC FIELDS

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The simultaneous effects of the electric and magnetic fields on the energy levels and optical properties of the GaAs pyramidal quantum dots are investigated within the density matrix formalism with the use of the effective mass and parabolic band approximations. Two different geometries with different values of the height-to-base length ratio were used to describe the electron behavior in the weak and strong confinement regimes, respectively. We obtained the energy levels and wave functions in the presence of electric field by using a variational method, whereas the magnetic field effect was estimated within the perturbational theory Our results suggest that the geometry and the external applied fields play an important role in the electronic and optical properties of a pyramid-shaped quantum dot.

Keywords: energy levels, optical properties, quantum dot

1. Introduction

The intersubband transitions and optical properties induced by interband and intersubband transitions [1-5] in semiconductor nanostructures have been extensively studied over the past decades. Among these systems, the quantum dots (QDs) are of great interest due to their prospective applications in the design and fabrication of optoelectronic devices [6-10]. Applying the external fields (electric/magnetic) may lead to significant modifications of the electron energy spectrum in quantum heterostructures. This certainly affects a large number of their properties. One of the most important consequences of the application of a static electric field is the possibility of obtaining rather strong nonlinear optical responses, resulting from the consequent increment in the expected values of the electron dipole moment, as it was originally shown by Ahn and Chuang in the case of quantum wells [11]. Regarding the magnetic fields, in general their contribution is to increase the carriers confinement due to the decrease of the

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cyclotron orbits radius with the applied field, leading to blue-shifts in the optical absorption and photoluminescence spectra [12].

The quantum dots of pyramidal shape have received a special attention due to their growing applications in different areas of modern science and technology (lasers, photonic structures, light detectors and solar cells; see, for example, Refs. [13-16]. Their theoretical treatment within the traditional quantum mechanical approach is mathematically difficult and, in fact, the system can be studied only by numerical techniques [17-19]. So, the search for analytical solutions of the problem, even solutions with certain restricted applicability, could be considered as an important and interesting research. For pyramidal dots with small values of the vertex angle and within the infinite quantum confinement approximation, Lozovski and Piatnytsia [20] have obtained electron energy structure and analytical expressions for the electron wave functions. The effect of the impurity positions on the linear and nonlinear intersubband optical absorption in a pyramid and a cone like quantum dot without applied external fields has been studied by Khordad and Bahramiyan [19]. They found that there is a maximum value of the total refractive index change and absorption coefficients at a special impurity position. The effect of QD structure parameter on the energy levels, dipole matrix element, absorption coefficient and third order susceptibilities are studied by Saghai et al. [21]. They used the 3D-finite difference model to solve the 3D Schrodinger equation, to calculate the electrical and optical properties of pyramid and prism QDs. However, there is no work on the effect of the external applied fields on the electronic and optical properties of such a structure.

In this work we calculated the energy levels and the modified wave functions for the ground and first excited states in pyramid shaped QDs under combined action of the electric and magnetic fields applied in the growth direction. The effects of the external applied fields on the linear intersubband optical absorption are also investigated. The paper is organized as follows. In Section 2 we describe the details of the theoretical approach. Section 3 is dedicated to the results and discussion, and finally, our conclusions are given in Section 4.

2. Theory and model

In the framework of the effective mass approximation, the Hamiltonian of an electron inside a pyramid-shaped QD with the square base $b \times b$ and the height h under external applied fields can be written as

$$\hat{H} = \frac{\left(\vec{p} + e\vec{A}\right)^2}{2m^*} + V\left(\vec{r}\right) + e\vec{F} \cdot \vec{r} \tag{1}$$

The first term of the Hamiltonian is the Kinetic term of the electron under the influence of the magnetic field $\vec{B}$, where m^* is the electron effective mass, e is the elementary charge, and $\vec{p}$ is the electron momentum operator. In the symmetric gauge, the vector potential $\vec{A}$ associated to the z-axis magnetic field is chosen as $\vec{A} = -(B/2)(-y\hat{x} + x\hat{y})$. Following Ref. [20] we consider an infinitely high potential barrier, i.e. $V(\vec{r})$ is zero inside the dot and infinitely otherwise. We choose the electric field oriented along the growth direction, $\vec{F} = F\hat{z}$ (see Fig. 1).

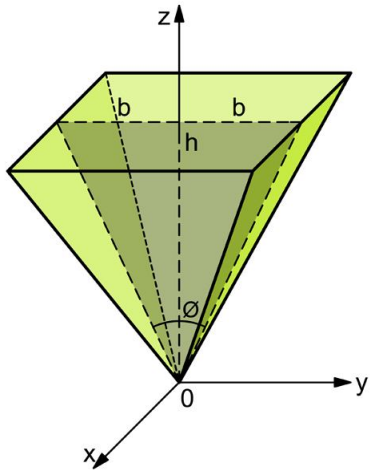

Fig. 1. The geometry of the pyramid-shaped quantum dot.

In the absence of the electric field the eigenfunctions and the eigenenergies of the Hamiltonian are obtained by using coordinate transformations shown by [22]:

$$u = x/z;\ v = y/z;\ w = z. \tag{2}$$

This change transforms the pyramid into a rectangular parallelepiped of rib length $2/a$ (where $a = \tan^{-1}(\phi/2)$, with ϕ the vertex angle of the pyramid) and height h. The parallelepiped boundaries are defined by:

$$u \in [-1/a, 1/a],\ \ v \in [-1/a, 1/a],\ \ w \in [0, h] \tag{3}$$

In the absence of the external applied fields the Schrödinger equation [20] becomes:

$$-\frac{\hbar^2}{2m^*}\Delta_{uvw}\psi = E_0\,\psi \tag{4}$$

where:

$$\Delta_{uvw}=\frac{1}{w^2}\left(\frac{\partial^2}{\partial u^2}+\frac{u}{u^2+v^2+1}\frac{\partial}{\partial u}\right)+\frac{1}{w^2}\left(\frac{\partial^2}{\partial v^2}+\frac{u}{u^2+v^2+1}\frac{\partial}{\partial v}\right)+\frac{1}{w^2\left(u^2+v^2+1\right)}\frac{\partial}{\partial z}\left(w^2\frac{\partial}{\partial w}\right) \tag{5}$$

In the small vertex angle approach $\phi<90^o$, so that $u,v<<1$, Eq. (4) can be reduced to an equation with separate variables and its solutions are expressed [20] as:

$$\psi_{pqr}(u,v,z)=\chi_p(u)\,\eta_q(v)\xi_r(w) \tag{6}$$

The wave functions $\chi_p(u)$ and $\eta_q(v)$ vanish in $\pm 1/a$ and they are given by

$$\chi_p(u)=C_1\sin\left(k_p a^{-1}\right)\cos\left(k_p u\right)+\cos\left(k_p a^{-1}\right)\sin\left(k_p u\right) \tag{7}$$

with $k_p=p\pi a/2$, p = 1,2, and

$$\eta_q(v)=C_2\sin\left(k_q a^{-1}\right)\cos\left(k_q v\right)+\cos\left(k_q a^{-1}\right)\sin\left(k_q v\right) \tag{8}$$

with $k_q=q\pi a/2$, *q=1,2,3...*, C_p being the normalization constants.

Finally, the function $\xi_r(w)$ is given by [20]:

$$\xi_r(w)=J_r\left(k_{pqr}w\right)/\sqrt{w} \tag{9}$$

where $J_r\left(k_{pqr}w\right)$ is the spherical Bessel function of order r and $r=\sqrt{k_p^2+k_q^2+1/4}$. The boundary conditions impose that

$$J_r\left(k_{pqr}h\right)=0 \tag{10}$$

where $k_{pqr}h$ represents the r^{th} zero of the Bessel function $J_r\left(k_{pqr}w\right)$. In Cartesian coordinates the unperturbed wave functions (WFs) associated to the lowest electron states [20] can be written as:

$$\psi_{111}(x,y,z)=J_{\upsilon_1}(k_{111}z)\cos\left(\frac{\pi a}{2}\frac{x}{z}\right)\cos\left(\frac{\pi a}{2}\frac{y}{z}\right)/\sqrt{z} \tag{11}$$

and

$$\psi_{112}(x,y,z)=J_{\upsilon_1}(k_{112}z)\cos\left(\frac{\pi a}{2}\frac{x}{z}\right)\cos\left(\frac{\pi a}{2}\frac{y}{z}\right)/\sqrt{z} \tag{12}$$

with $\upsilon_1=\sqrt{2(\pi a/2)^2+1/4}$.

When an electric field is applied in the growth direction the simple form of the trial wave function:

$$\Phi_1=N_1\psi_{111}\exp(-\lambda_1 z) \tag{13}$$

where N_1 is the normalization constant, gives accurate results for the ground state [23]. To find an analytic form for the first-excited state within the same variational procedure, we used the Gram-Schmidt orthogonalization procedure [23]. This

procedure requires the construction of an orthonormal set $\{\Phi_1, \Phi_2, ...\}$ from an independent set $\{\Psi_{pqr}(z)\exp(-\lambda_{pqr}z)\}$ which is not orthonormal.

The corresponding wave function for the first-excited state (which is orthogonal to Φ_1 state) can be written as:

$$\Phi_2 = N_2\left[\psi_{112}\exp(-\lambda_2 z) - \langle\psi_{112}\exp(-\lambda_2 z)|\Phi_1\rangle\Phi_1\right] \tag{14}$$

Here N_2 is the normalization constant and $\langle\psi_{112}\exp(-\lambda_2 z)|\Phi_1\rangle$ is the inner product between the involved WFs. The calculation of the wave functions and energy levels when there is a non-zero applied magnetic field leads to the use of the perturbation theory in the non-degenerate case (zero-order corrections to the wave functions and first-order corrections to the energies). Finally, we used the perturbed electron states to investigate the linear optical absorption in GaAs pyramid-shaped QDs under external fields for two cases: (a) in a weak confinement regime, for a quantum dot with $b = 50$ nm and $h = 50$ nm and (b) in a strong confinement regime, for a quantum dot with $b = 26$ nm and $h = 16$ nm. Note that nanodots with such sizes have been obtained by the selective epitaxial growth on masked substrates by metalorganic chemical vapor deposition [24] and by Droplet Epitaxy on Ge virtual substrates, respectively [25].

If the system under study is excited by an electromagnetic field of frequency ω linearly polarized along the *z*-axis, we may write the electric-dipole matrix element as:

$$M_{12} = e\langle\Phi_1|z|\Phi_2\rangle \tag{15}$$

where $\Phi_1(z)$ and $\Phi_2(z)$ are given by the equations (13) and (14).

Using density matrix formalism and neglecting the higher harmonic terms, the linear susceptibility is connected to the dipole matrix element [24] by:

$$\varepsilon_0\chi^{(1)}(\omega) = \frac{\sigma|M_{12}|^2}{\Delta E - \hbar\omega - i\hbar/\tau_{in}} \tag{16}$$

where σ is the electron density of the QD, $\Delta E = E_2 - E_1$ is the transition energy for the perturbed system and $\hbar/\tau_{in}$ is the damping term associated with the lifetime of the electrons due to intersubband scattering.

The imaginary part of susceptibility, $\mathrm{Im}\,\chi$, determines the absorptive spectrum and the real part, $\mathrm{Re}\,\chi$, is related to the refractive index as follows:

$$n(\omega) = 1 + \frac{1}{2}\,\mathrm{Re}\,\chi(\omega) \tag{17}$$

In the next section we present our results for the electronic states and optical properties in GaAs QDs taking into account the combined effects of the external applied fields and the quantum confinement.

3. Results and discussion

The previous studies [26,27], have shown that the properties of the pyramidal dots, such as transition energy, transition dipole moment, oscillator strength, and susceptibility, are not only sensitive to QD size, but also they are highly sensitive to height-to-base length ratio h/b. So, we investigated the linear optical absorption in GaAs pyramid-shaped QDs under external fields for the two abovementioned cases, referred to in the following as QD1 and QD2.

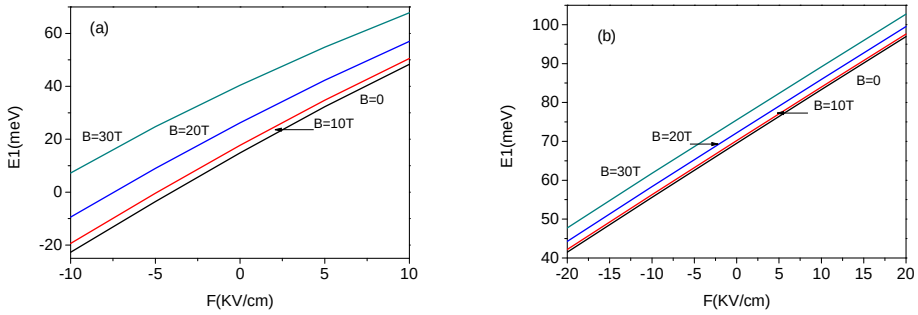

Fig.2. The ground state energy as a function of the electric field for (a) QD1 and (b) QD2 structure. Several values of the magnetic field are considered.

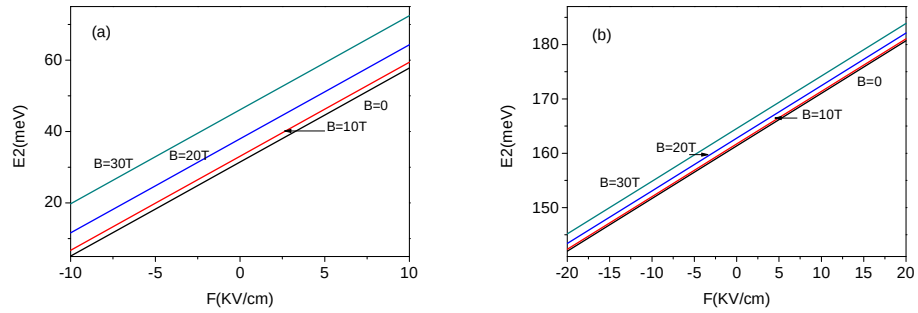

Fig.3. The results are as in Fig. 2, but for the first excited state of the electron.

In Fig. 2 we presented our results for the ground state energy of the electron as function of the electric field for several magnetic field strengths for (a) QD1 and (b) QD2 structures, whereas Fig. 3 shows the results for the first excited state.

As expected, for $F > 0$ the electron energy increases for both pyramids because the wave functions are pushed towards the top of the pyramid-shaped dot

and they become strongly compressed by the potential barriers. As a consequence, there is an increasing of the kinetic energy, more pronounced for the QD1 structure where the electric field effect is the predominant over the effect of the quantum confinement. On the other hand, negative electric fields move the electron cloud towards the pyramid base where the barrier effects are diminished, leading to smaller kinetic energies. It is also observed an enhancement of the energies as B increases as a result of the supplementary magnetic field confinement on the electron.

The energy difference between the first excited state and the ground state $\Delta E = E_2 - E_1$ which is proportional to transition frequency has been calculated in function of the electric applied field for several B values and is presented in Fig. 4. We note that: (i) the smaller dot case (QD1) leads to a higher transition frequency; (ii) this quantity decreases with the increasing electric and magnetic fields.

The interesting fact is that the application of a positive electric field yields a red-shift in the transition energy, while an electric field oriented towards the pyramid's top induces a blue-shift in the transition energy. As expected, in the strong confinement regime (Fig. 4b) the transition energy is less sensitive to the magnetic field variation.

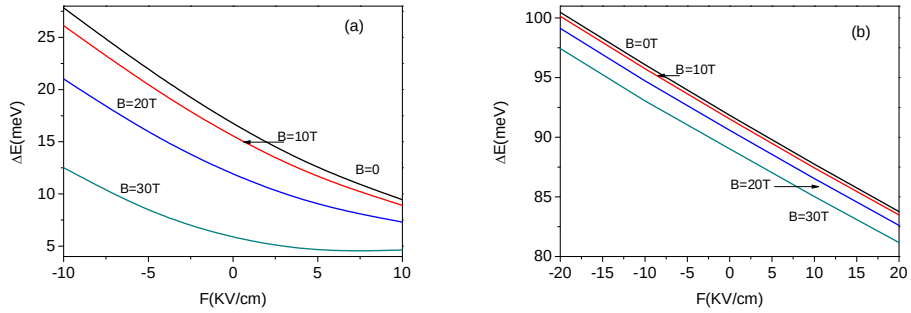

Fig.4. The transition energy as a function of the electric field for (a) QD1 and (b) QD2 structure. Several values of the magnetic field are considered.

To complement the dc field effects on the electronic structure, and provide a ground for the discussion of the optical properties below, in Fig. 5 we plotted the variation of the dipole matrix element M_{12}.

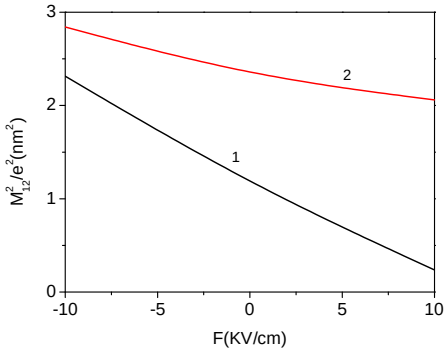

Fig.5. The dipole matrix element as a function of the electric field. Numbers (1) and (2) are for QD1 and QD2, respectively.

The decreasing of this quantity with the applied electric field relates to the increase of the field-induced separation of the wave functions involved in the optical transition. In the zero-electric field, the overlapping between WFs occurs mainly in the central region of the QD. As long as F strengthens, the eigenfunction corresponding to the upper state of the transition will suffer a stronger displacement towards the top of the dot, leading to a lower degree of overlap with the lower one. A similar behavior of the dipole matrix element has been reported in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells for lower values of the electric field [28].

Figs. 6 and 7 show both the real and the imaginary parts of the linear susceptibility as a function of the photon frequency for the structures in our research.

The results are for some values of F, with and without applied magnetic field. According to Fig. 4, the resonance frequency $\omega_r = \Delta E/\hbar$ shows a red-shift when the external electric field is applied along the z-direction and a blue-shift for F oriented towards the pyramid's top as mentioned above. Thus, the absorption and dispersion curves move towards the lower frequency together with the increase of the $|\vec{F}|$ value and this effect is more pronounced for QD1 structure.

On the other hand, for this quantum dot we can observe an important reduction of the magnitude of $\mathrm{Re}\,\chi(\omega)$ and $\mathrm{Im}\,\chi(\omega)$ (quantities directly proportional to the square of dipole matrix element and roughly inversely proportional to the square of ΔE). This effect mainly results from the decrease in M_{12}^2 induced by the electric field, because the overall effect of augmenting F on the fundamental transition energy is to reduce its value (see Fig. 4). As expected, the values of the peak show a smaller decrease in the QD2 due to the stronger quantum confinement permitted by this structure in comparison with QD1.

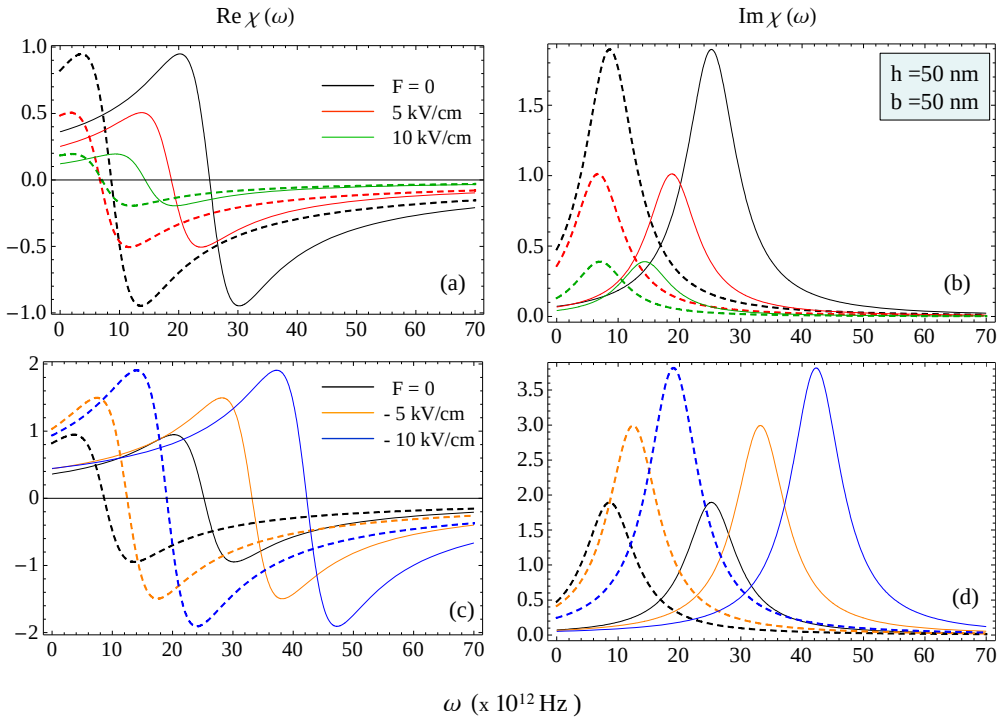

Fig.6. Real (left column) and imaginary (right column) parts of susceptibility as functions of incident light frequency ω for the QD1 structure. Several values of the applied electric field are considered. Solid and dotted lines are for $B = 0$ and $B = 30$ T, respectively.

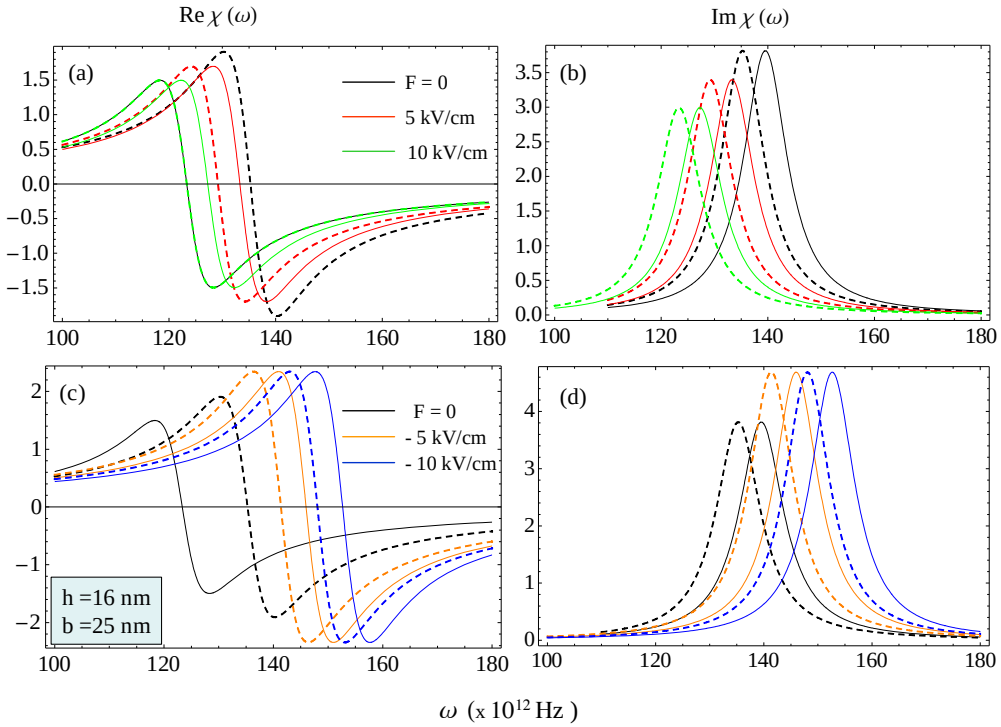

Fig.7. As in Fig. 6, for the QD2 structure.

6. Conclusions

The electronic properties and absorption spectra for electrons confined in pyramid-shaped QDs with different values of the height-to-base length ratio under simultaneous action of the electric and magnetic applied fields have been investigated. We found that, depending on the direction of the applied electric field, a significant blue or red shift of the energy levels is obtained and its magnitude may be tuned by the supplementary magnetic confinement. Our calculations revealed that the main parameters that affect optical absorption are the dot size and the electric field, but this can be also controlled by using an external magnetic field.

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