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# Electron-related linear and nonlinear optical responses in vertically coupled triangular quantum dots

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ABSTRACT

The conduction band states of GaAs-based vertically coupled double triangular quantum dots in two dimensions are investigated within the effective mass and parabolic approximation, using a diagonalization procedure to solve the corresponding Schrödinger-like equation. The effect of an externally applied static electric field is included in the calculation, and the variation of the lowest confined energy levels as a result of the change of the field strength is reported for different geometrical setups. The linear and nonlinear optical absorptions and the relative change of the refractive index, associated with the energy transition between the ground and the first excited state in the system, are studied as a function of the incident light frequency for distinct configurations of inter-dot distance and electric field intensities. The blueshift of the resonant absorption peaks is detected as a consequence of the increment in the field intensity, whereas the opposite effect is obtained from the increase of inter-dot vertical distance. It is also shown that for large enough values of the electric field there is a quenching of the optical absorption due to field-induced change of symmetry of the first excited state wavefunction, in the case of triangular dots of equal shape and size.



## 1. Introduction

The two-dimensional triangular geometry in quantum confined systems has been investigated with particular emphasis since the advent of semiconductor-based nanostructures. Mathematical aspects of the exact solution of the non-separable Schrödinger problem of particles completely confined in equilateral and isosceles triangles were put forward in the eighties of last century [1–4]. Gangopadhyay and Nag approached the calculation of the energy spectrum of electrons in finite barrier height quantum wires of triangular shape by expanding the wavefunctions in terms of the eigenfunctions of a system with right-angle isosceles triangular shape and infinite barrier height [5]. The direct numerical solution that uses finite-element method allowed us to determine the electron states in GaAs-based triangular quantum dots (QDs) in the presence of magnetic fields [6]. A few years ago, Khordad et al. reported the intersubband-related optical response of electrons in infinite-barrier quantum wires with equilateral triangular cross-section [7–9]. On the other hand, there are also reports on the practical realization of metallic, dielectric and semiconducting nanostructures bearing the triangular geometry. Among the more recent one we can mention the works of references [10–13].

The investigation on the linear and the nonlinear optical absorption in a quantum well under the influence of an externally applied static electric field appeared for the first time in a work by Ahn and Chuang [14]. They proposed the calculation of the dielectric susceptibility via a perturbative solution of Von Neumann's equation for the density matrix and derived this kind of expressions that, thereafter, have been used throughout the years in evaluating the light absorption coefficients due to intersubband transitions in quantum nanostructures. The same kind of mathematical procedure – but instead of taking the real part of the susceptibility – leads to the corresponding expressions for the relative change of the refractive index. In the case of the triangular-shaped systems, one finds, for instance, the report on these particular optical responses by Khordad et al. [7] and the study of impurity-related optical absorption and relative refractive index change by Duque et al. [15], in quantum wires of triangular cross-section.

In the present work we are aiming for presenting a study of electron states and the related linear and nonlinear light absorptions and the changes in the index of refraction due to intersubband transitions in vertically arranged coupled two-dimensional

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triangular quantum dots with finite confining barrier height. In addition, the structure will be considered under the influence of an external DC electric field. The organization of the work is as follows: Section 2 contains the details of the used theoretical approach. Section 3 is devoted to the presentation and discussion of the obtained results, whereas the corresponding conclusions appear in the last section.

## 2. Theoretical framework

In this work we investigate the conduction band states of a double two-dimensional triangular potential well system coupled by an electric field applied along the $y$-direction, by working in the effective mass and parabolic approximations.

The particular symmetry of the confining potential suggests that, in the mathematical description of the system, we use the Cartesian coordinates. In accordance, the two-dimensional single-band Hamiltonian is given by

$$H=-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]+V(x,y), \tag{1}$$

where $m^*$ is the electron effective mass, and $V(x,y)$, the 2D potential, responsible for the charge carrier confinement, is schematically depicted in Fig. 1.

In order to solve the Schrödinger-like equation with the Hamiltonian equation (1) we propose the single electron wavefunction in the form of a two-dimensional expansion over the orthonormal set of sinusoidal basis functions arising from the solution of a 2D rectangular infinite potential well of sides $L_x \times L_y$. Hence, we can write

$$\Psi(x,y)=\frac{2}{\sqrt{L_xL_y}}\sum_{m,n}C_{m,n}\ \sin\left[\frac{m\pi x}{L_x}+\frac{m\pi}{2}\right]\ \sin\left[\frac{n\pi x}{L_y}+\frac{n\pi}{2}\right], \tag{2}$$

where $m=1,2,\ldots$ and $n=1,2,\ldots$. This proposal turns the problem of solving the differential equation into the diagonalization of an infinite Hamiltonian matrix. For practical purposes in our calculation we have considered 225 terms in the expansion.

Taking into account the obtained electronic structure, and considering a $y$-polarization for the incident radiation, it is possible to evaluate the expressions for the linear and third order nonlinear optical absorption coefficients. In our case, this is accomplished by using the density matrix approach for obtaining the electronic polarization, **P**, as a response to a harmonically time dependent electric field, **E**, of frequency $\omega$ [14,16,17]:

$$P(t)=\frac{1}{S}\mathrm{Tr}[\hat{\rho}\hat{M}]=\chi(\omega)E(t), \tag{3}$$

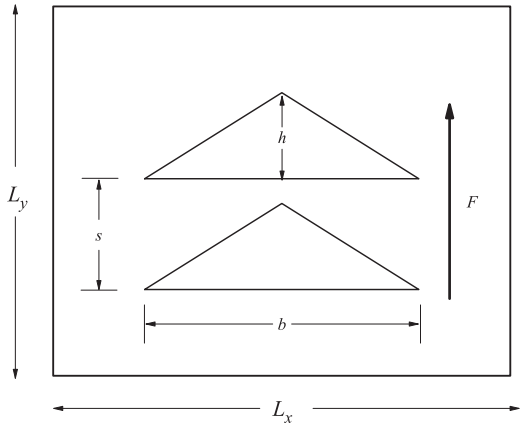


**Fig. 1.** Pictorial view of the potential profile of two 2D triangular quantum dots coupled by means of an electric field ($F$) applied along the $y$-direction.

where $\hat{\rho}$ is the statistical operator, $\hat{M}$ the electric dipole moment operator, $\chi(\omega)$ the dielectric susceptibility, and $S$ the total area of the system. Then, one can derive the optical absorption coefficients from the imaginary part of the dielectric susceptibility. According to Ahn and Chuang, and Takagahara [14,16], for enough small values of the incident light intensity ($I$) it is possible to use the usual approach for solving Von Neumann's equation for $\hat{\rho}$ via a multi-order expansion. In the process, we would be able to evaluate the electric dipole moment transition matrix element $M_{01}=\langle\Psi_0|y|\Psi_1\rangle$, where 0 and 1 generically represent the initial and the final state of the transition. This procedure leads to the following expression for the linear contribution:

$$\alpha^{(1)}(\omega)=\omega e^2\sqrt{\frac{\varepsilon}{\mu}}\left[\frac{\rho\hbar\Gamma_{01}|M_{01}|^2}{(E_{10}-\hbar\omega)^2+(\hbar\Gamma_{01})^2}\right]. \tag{4}$$

Meanwhile, the intensity-dependent third order correction is

$$\alpha^{(3)}(\omega,I)=-\omega e^4\sqrt{\frac{\varepsilon}{\mu}}\left(\frac{I}{2n\varepsilon_0c}\right)\frac{\rho\hbar\Gamma_{01}|M_{01}|^2}{[(E_{10}-\hbar\omega)^2+(\hbar\Gamma_{01})^2]^2}\times\left\{4|M_{01}|^2-\frac{|M_{11}-M_{00}|^2[3E_{10}^2-4E_{10}\hbar\omega+\hbar^2(\omega^2-\Gamma_{01}^2)]}{E_{10}^2+(\hbar\Gamma_{01})^2}\right\}, \tag{5}$$

$$\alpha(\omega,I)=\alpha^{(1)}(\omega)+\alpha^{(3)}(\omega,I). \tag{6}$$

On the other hand, the linear and nonlinear coefficients of the relative change of the refractive index in the system are proportional to the corresponding real parts of the first- and third-order contributions to the dielectric susceptibility. In accordance, we will have

$$\frac{\Delta n^{(1)}(\omega)}{n_r}=\frac{e^2\rho|M_{01}|^2}{2n_r^2\varepsilon_0}\frac{E_{10}-\hbar\omega}{(E_{10}-\hbar\omega)^2+(\hbar\Gamma_{01})^2}, \tag{7}$$

in the case of the first-order term, whereas the third-order correction is given by

$$\frac{\Delta n^{(3)}(\omega)}{n}=-\frac{\rho e^4|M_{01}|^2}{4n^3\varepsilon_0}\frac{\mu cI}{[(E_{10}-\hbar\omega)^2+(\hbar\Gamma_{01})^2]^2}\times\left[4(E_{10}-\hbar\omega)|M_{01}|^2-\frac{(M_{11}-M_{00})^2}{(E_{10})^2+(\hbar\Gamma_{01})^2}\{(E_{10}-\hbar\omega)\times[E_{10}(E_{10}-\hbar\omega)-(\hbar\Gamma_{10})^2]-(\hbar\Gamma_{01})^2(2E_{10}-\hbar\omega)\}\right]. \tag{8}$$

The total relative change of the refractive index is the sum of these two contributions:

$$\frac{\Delta n(\omega,I)}{n_r}=\frac{\Delta n^{(1)}(\omega)}{n_r}+\frac{\Delta n^{(3)}(\omega,I)}{n_r}. \tag{9}$$

In the expressions (4) and (5) and (7) and (8), the quantity $E_{10}=E_1-E_0$ is the transition energy difference between the two lowest allowed energy levels. Besides, $e$ is the elementary charge, $\mu$ is the magnetic permeability of vacuum, $\varepsilon_0$ is the free-space dielectric permittivity, and $c$ is the speed of light in vacuum. The $\Gamma_{01}$ is the dephasing intersubband damping rate, and $\rho=(\rho_{00}-\rho_{11})/S$ is the 2D density of carriers involved in the transition (with $\rho_{ij}$ representing the equilibrium occupation number of the $j$-th state). Finally, $n_r=\sqrt{\varepsilon}$ is the refractive index of the material in the active region of the structure. Our prototype structure is made of $GaAs$ triangular regions embedded into an $Al_xGa_{1-x}As$ rectangular region, with $Al$ molar fraction of $x=0.3$. In this context, the value of the potential within the triangle regions is $V_i(x,y)=0$ and, considering a valence band offset for the $Al_xGa_{1-x}As$ of 0.6, the potential outside the triangular quantum dots is $V_o(x,y)=228$ meV. The remaining set of input parameters are the conduction electron effective mass $m^*=0.067\,m_0$ (being $m_0$ the free electron mass); the static relative dielectric constant is chosen to be $\varepsilon_r=12.58$. Then, the effective GaAs Bohr radius is $a_0^*=99.36$ Å and the effective Rydberg is $Ry^*=5.76$ meV. The setup for the