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Electron-related optical responses in triangular quantum dots

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HIGHLIGHTS

- Optical absorption and changes in refractive index in triangular quantum dots.
- The effective mass and parabolic band approximations have been used.
- The increase in the size of the dot leads to a red shift of optical properties.
- Also, an increment in the values of the off-diagonal electric dipole moment matrix.
- The increase of the amplitude of the optical absorption is observed.

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ABSTRACT

The linear and nonlinear coefficients for the optical absorption and relative refractive index change associated with intersubband transitions of electrons in the conduction band of a two-dimensional quantum dot of triangular shape are calculated for *x*-polarization and *y*-polarization of the incident light. Both the effective mass and parabolic band approximations have been considered. The results show that the increase in the size of the triangular quantum dot leads to the expected fall of the intersubband energy transition and that there is an increment in the values of the associated off-diagonal electric dipole moment matrix elements. All this reflects in the increase of the amplitude of the nonlinear optical absorption resonant peak, as well as in the growth of the total relative refractive index in the system.

1. Introduction

Many studies on the fundamental properties and applications of low-dimensional semiconductor structures (LDSS) have been carried out for more than four decades. To obtain a brief account of them we can, for instance, refer to the book by Harrison (and the number of references therein) [1]. Many physical properties related with the effect of the carrier states confinement exhibit particular – or even unusual – features in this kind of systems. In the particular case of the quasi-zero-dimensional structures known as quantum dots (QDs), comprehensive reviews of their electronic and optical properties are provided in the works by Yoffe [2] and Reimann and Manninen [3].

The triangular geometry is the one usually considered in the theoretical modeling of the confining profile in the conduction and valence band of quantum nanostructures. However, for specific materials and growth conditions, the triangular shape also relates with the more favorable free energy configuration. Accordingly, there are reports on the practical realization triangularly shaped metallic, dielectric and semiconducting. Some of the more recent appear in Refs. [4–7]. The solution of the Schrödinger-like problem in triangularly confined systems has the peculiarity of being non-separable. In consequence, different attempts of providing exact solving for the eigenstates have taken advantage of particular triangular geometries and their associated inherent symmetries. The exact solution of the Schrödinger equation for a particle completely confined to an equilateral triangle was given, for instance, by Krishnamurthy et al. [8]. The use of projection operators and group theory allowed Li to obtain the energy levels and wavefunctions in right isosceles [9] and equilateral [10,11]

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triangles. A problem with finite barrier height in triangular and arrowhead-shaped quantum wires was approached by using the eigenfunctions of an infinite-barrier right-angled isosceles triangular wire [12], and a finite-element method allowed to determine the eigenstates of electrons in GaAs QDs of triangular shape in the presence of magnetic fields [13].

The nonlinear optical properties of LDSS have been a subject of much interest in the past years [14]. In these structures, the rather large values of the oscillator strength are responsible for the appearance of high dipole moment expectation values, which manifest through pretty high nonlinear optical responses. Among the somewhat extensive literature on the subject, we may refer, for instance, to the experimental observation of second harmonic generation [15,16], the third harmonic generation [17], and the four wave mixing [18]. There are also many theoretical studies regarding optical nonlinearities in semiconductor heterostructures, among which we may cite the set of Refs. [19–32].

Khordad and collaborators have published a number of articles which report on the intersubband-related optical response of semiconducting GaAs-based quantum well wires (QWWs) of triangular- and parallelogram-shaped cross section with infinite lateral potential barriers [33–35]. Exact eigenfunctions of a QWW with equilateral triangular cross section were used in Ref. [33] in the calculation of the nonlinear optical absorption and the relative change in the refractive index. Generation of second and third order harmonics is the subject of research in Ref. [35]. For the purpose of such studies, these authors chose a suitable configuration of initial and final states for the intersubband electronic transitions which corresponds to considering only a particular subset of the complete set of eigenstates otherwise obtained by Li and Blinder for the equilateral triangle problem [10].

With all this in mind, the aim of the present work is to present the results of the study of the linear and nonlinear optical absorption and relative change of the refractive index coefficients associated with intersubband electron transitions in a two-dimensional (2D) QD of equilateral triangular shape and finite confinement potential. Our method for calculating the single-electron states within the effective mass and parabolic band approximations uses the exact diagonalization of the Hamiltonian matrix obtained from the Fourier-like expansion of the conduction band wavefunctions in terms of the complete set of eigenstates corresponding to a rectangular — infinite barrier — potential configuration. The organization of the work is as follows: Section 2 briefly presents the description of the theoretical model. In Section 3 one finds the corresponding results and discussion. Finally, Section 4 contains the main conclusions of the study.

2. Theoretical framework

The model quantum dot has a triangular shape with equal sides of length L (for illustration, see Fig. 1). We use the effective mass and parabolic approximations to describe the conduction band states and choose the Cartesian coordinates for writing the two-dimensional Hamiltonian

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

where m^* is the electron effective mass and $V(x,y)$, the confining 2D potential;

$$V(x,y)=\begin{cases}0 & \text{if } (x,y) \text{ lies within the dot region;}\\ V_0 & \text{if } (x,y) \text{ lies outside the dot region,}\end{cases} \tag{2}$$

whilst the region limited by the triangle is given by $(x_1 \le x \le x_3 \wedge y_1 \le y \le k_1) \cup (x_3 < x \le x_2 \wedge y_1 \le y \le k_2)$, where $k_1 = y_1 + m_1(x-x_1)$, $k_2 = y_2 + m_2(x-x_2)$, $x_1=-L/2$, $x_2=+L/2$, $x_3=0$, $y_1=y_2=-L\sqrt{3}/6$, $y_3 = L\sqrt{3}/3$, $m_1=(y_3-y_1)/(x_3-x_1)$, and $m_2=(y_3-y_2)/(x_3-x_2)$.

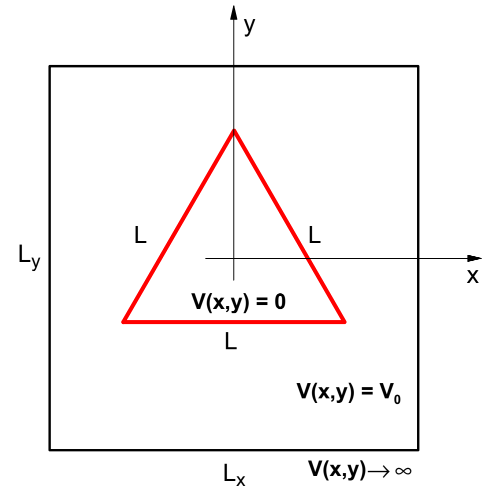

Fig. 1. Pictorial view of the equilateral triangular quantum dot considered in the present work. The values of the confinement potential are shown for the three different regions of the problem. The auxiliary rectangular area used to generate the orthonormal set of basis functions for the Fourier expansion of the eigenstates is depicted as well.

We propose the solution of the two-dimensional effective mass equation for the confined motion of the electron via a 2D Fourier expansion in the region corresponding to a rectangle of dimensions $L_x \times L_y$ (see Fig. 1). The complete set of basis functions is a product of sine-like functions, which are the eigenstates of the corresponding Schrödinger-like problem with energies

$$E_{m,n}=\frac{\hbar^2\pi^2}{2m^*}\left(\frac{m^2}{L_x^2}+\frac{n^2}{L_y^2}\right). \tag{3}$$

Accordingly, we may write

$$\Psi(x,y)=\frac{2}{\sqrt{L_xL_y}}\sum_{m,n}C_{m,n}\,\sin\left[\frac{m\pi(x+L_x/2)}{L_x}\right]\sin\left[\frac{n\pi(y+L_y/2)}{L_y}\right], \tag{4}$$

where $m=1,2,\ldots$ and $n=1,2,\ldots$. This proposal turns the problem of solving the differential equation (1) into the diagonalization of an infinite Hamiltonian matrix. For practical purposes in our calculation we have considered 225 terms in the expansion. We have found that this ensures a suitable convergence and the appropriate wavefunction normalization.

With these states, and for w-polarization ($w=x,y$) of the incident radiation, we can derive the expressions for the coefficients of linear and nonlinear optical responses through the calculation of the dielectric susceptibility in the system. This is accomplished with the use of the density matrix approach for obtaining the electronic polarization, **P**, as a response to an electromagnetic field **E** of frequency ω [20,36,37]. Then, we need to evaluate

$$P(t)=\frac{1}{S}\mathrm{Tr}[\hat{\rho}\hat{M}]=\chi(\omega)E(t), \tag{5}$$

where $\hat{\rho}$ is the statistical operator, $\hat{M}$ is the electric dipole moment operator, $\chi(\omega)$ is the dielectric susceptibility, and S is the total area of the system. In the process, we shall be able to evaluate the electric dipole moment transition matrix element $M_{fi}=\langle\Psi_f|w|\Psi_i\rangle$. For small enough values of the incident light intensity it is possible to use the usual procedure of solving Von Neumann's equation for $\hat{\rho}$ by means of a multi-order expansion. It allows for obtaining of the dielectric susceptibility, the expressions for these quantities are [36,37]

$$\alpha^{(1)}(\omega)=\omega\sqrt{\frac{\mu}{\epsilon_r}}\frac{e^2\sigma\hbar\Gamma_{if}|M_{fi}|^2}{(E_{fi}-\hbar\omega)^2+(\hbar\Gamma_{if})^2} \tag{6}$$