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Properties of the second and third harmonics generation in a quantum disc with inverse square potential. A modeling for nonlinear optical responses of a quantum ring

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ABSTRACT

The calculation of the second and third harmonic generation coefficients is carried out within the framework of the effective mass approximation in two-dimensional GaAs quantum discs under the combined effect of an external magnetic field and parabolic and inverse square confining potentials. Due to the electric dipole selection rules, the system is shown to have second harmonic generation coefficient identically zero for all the values of incident frequency. The generation of third optical harmonics is significantly dependent on the values of the different input parameters, with the presence of resonant peak blueshifts associated with the magnitudes of the parabolic confinement and the applied magnetic field.

1. Introduction

The application of self-assembly crystal growth techniques has made possible to fabricate quantum dot (QD) and quantum ring (QR) semiconductor structures (see, for instance, Ref. [1]). Both QD and QR systems are subjects of great interest due to their prospective applications in the design and production of optoelectronic devices [2–5]. Among the optical properties studied in this kind of nanostructures, the generation of second and third harmonics are of particular interest given the possibility of obtaining significant enhancements of the corresponding resonant peak amplitudes, compared with other low-dimensional systems and bulk materials [6,7]. Besides, the second harmonic generation (SHG) was experimentally detected in InAlGaAs QDs with the use of near-field optical scanning microscopy [8]. It is possible to mention several recent works on the subject. They consider SHG and/or third-harmonic generation (THG) in GaAs-based QDs with different geometries and confining potential profiles, with or without the inclusion of external electric and magnetic fields, as well as incorporating hydrostatic pressure or excitonic effects [9–16].

There is a particular type of quasi-zero-dimensional system known as quantum disc (QDC)—or disc-shaped quantum dot—which has also attracted some attention [17–19]. That is precisely the type of system we are dealing with the present article. A recent study on the so-called pseudo-QD which uses a two-dimensional pseudo-harmonic potential in cylindrical coordinates together with a magnetic field [20], can be considered as a precursor of the present one. Here, we are devoted to the study of the electronic states in two-dimensional quantum discs under a combination of two distinct confining profiles: a parabolic-type and the one provided by a potential energy function with inverse square dependence. All these are complemented with the presence of an externally applied magnetic field. The inverse square potential function appeared in the study of the quantum problem of N particles in a two-dimensional parabolic potential under a magnetic field [21]. We have already discussed that the use of this particular interaction, together with the other two potential field influences, leads to a rather direct modeling for the states of carriers confined in a two-dimensional semiconducting QR [22] (prior to the cited paper [22], Liu et al. have published an article on the electronic properties of quantum discs plus inverse squared potentials in which the authors report for the first time the basic equations of the model calculation [23]). The single electron eigenstates of the corresponding Schrödinger-like conduction band effective mass equation can be exactly described via analytical expressions in this case. As an application of the obtained energy levels and wavefunctions, we calculate the coefficients of SHG and THG in a GaAs-based system with such a geometry. The paper is organized as follows. In Section 2 we describe the theoretical framework. Section 3 is dedicated to the

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discussion of the obtained results, and our conclusions are given in Section 4.

2. Theoretical framework

A suitable set of coordinates for the description of the allowed quantum states of a confined electron in a disc shaped quantum dot (DSQD) is the polar system (r,φ). Including the presence of a static magnetic field **B**, oriented along the positive normal to the plane (here taken as the z-direction), the effective mass Hamiltonian of the system, is given by

$$H=\frac{1}{2m^*}\left[\mathbf{p}+\frac{q}{c}\mathbf{A}\right]^2+\frac{1}{2}m^*\omega_0^2r^2+\frac{\hbar^2}{2m^*}\frac{\lambda}{r^2}, \tag{1}$$

where $\mathbf{A}=(A_r=0,A_\varphi=Br/2,A_z=0)$ is the vector potential of the static magnetic field and q, m^* and c are the absolute value of the electron charge, the electron effective mass, and speed of light, respectively. Furthermore, ω_0 represents the frequency-like parameter used to describe a parabolic confinement potential (which is proportional to the external radius of the DSQD), whereas $\lambda\geq 0$ characterizes the strength of the repulsive inverse squared potential function. There will be a spatial region in the disc shaped quantum dot in which the repulsive effect of the potential barrier centered at the origin is strong enough to keep the electrons far from reaching values of the radial component close to $r=0$. This means that the behavior of the carrier system will largely resemble that of the electrons confined in a quantum ring. Accordingly, with a suitable combination of both ω_0 and λ, the model under consideration would be useful to simulate the electron spectrum in actual QRs, provided the advantages of having analytical expressions for both the wave functions and eigenvalues of the problem.

In the Coulomb gauge, the Schrödinger equation in polar coordinates has the form

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right)+\frac{1}{2}m^*\Omega^2r^2+\frac{\hbar^2}{2m^*}\frac{\lambda}{r^2}+\frac{\omega_c}{2}L_z\right]\psi=E\psi. \tag{2}$$

In this expression, $\omega_c=qB/m^*c$—known as the cyclotron frequency—and we have defined $\Omega=\sqrt{\omega_0^2+\omega_c^2/4}$ as the total confinement frequency in the magnetic field. E represents the energy eigenvalue, and L_z is the orbital angular momentum operator along the z-direction, respectively.

It is straightforward to show that the eigenfunctions of Eq. (2) are proportional to the so-called associated Laguerre polynomials [22,23]:

$$\psi(r,\varphi)_{mn}=\frac{N_{mn}}{\sqrt{r}}r^{2s_m}e^{-r^2/2\eta^2}L_n^{2s_m-1/2}(r^2/\eta^2)e^{im\varphi}, \tag{3}$$

where N_{mn} is the normalization constant. For details of calculations and definitions there, see for example Ref. [22]. The corresponding energy spectrum of the confined states is

$$E_{mn}=(2n+1+\sqrt{\lambda+m^2})\hbar\sqrt{\omega_0^2+\frac{\omega_c^2}{4}}+\frac{m\hbar\omega_c}{2} \tag{4}$$

with $n=0,1,2,\ldots$ and $m=0,\pm1,\pm2,\ldots$.

Given that some intersubband energy intervals, together with their corresponding dipole matrix elements, will be used to calculate the nonlinear optical coefficients for SHG and THG, we will choose here the energy levels and the wave functions participating in the transition as

$$E_0=E_{00},\quad E_1=E_{10},\quad E_2=E_{01},\quad E_3=E_{11} \tag{5}$$

and

$$\psi_0=\psi_{00},\quad \psi_1=\psi_{10},\quad \psi_2=\psi_{01},\quad \psi_3=\psi_{11}, \tag{6}$$

hence, we can express the quantities ω_{ij} as

$$\omega_{ij}=\frac{E_i-E_j}{\hbar}. \tag{7}$$

In particular, we focus on the frequency differences ω_{10}, $\omega_{20}/2$ and $\omega_{30}/3$, which are given respectively by

$$\omega_{10}=\left(\frac{1}{\sqrt{\lambda+1}+\sqrt{\lambda}}\right)\sqrt{\omega_0^2+\frac{\omega_c^2}{4}}+\frac{\omega_c}{2}, \tag{8}$$

$$\frac{\omega_{20}}{2}=\sqrt{\omega_0^2+\frac{\omega_c^2}{4}} \tag{9}$$

and

$$\frac{\omega_{30}}{3}=\frac{1}{3}\left(2+\frac{1}{\sqrt{\lambda+1}+\sqrt{\lambda}}\right)\sqrt{\omega_0^2+\frac{\omega_c^2}{4}}+\frac{\omega_c}{6}. \tag{10}$$

Finally, considering x-polarized monochromatic incident radiation interacting with the DSQD–QR, the electric dipole transition matrix elements are written as

$$M_{ij}=|\langle\psi_i|r\cos\varphi|\psi_j\rangle|. \tag{11}$$

At this point it is necessary to stress that, as a consequence of the electric dipole selection rules, the only non-zero matrix elements are those in which the magnetic quantum numbers involved in the transition have the following condition:

$$m-m'=\pm1. \tag{12}$$

Using the compact density matrix method and following an iterative procedure, the SHG and THG coefficients due to intersubband transitions in a DSQD–QR are given, respectively, by [16,24,25]

$$\chi^{(2)}_{2\omega}(\omega)=\frac{\sigma_\nu e^3}{\epsilon_0\hbar^2}\frac{M_{01}M_{12}M_{20}}{(\omega-\omega_{10}-i\Gamma_0)(2\omega-\omega_{20}-i\Gamma_0/2)} \tag{13}$$

and

$$\chi^{(3)}_{3\omega}(\omega)=\frac{\sigma_\nu e^4}{\epsilon_0\hbar^3}\frac{M_{01}M_{12}M_{23}M_{30}}{(\omega-\omega_{10}-i\Gamma_0)(2\omega-\omega_{20}-i\Gamma_0/2)(3\omega-\omega_{30}-i\Gamma_0/3)}, \tag{14}$$

where σ_ν is the electron density of the DSQD–QR, e is the electron charge, ϵ_0 is the vacuum permittivity, and $\hbar\omega$ is the incident photon energy.

Taking into account the condition given by Eq. (12) we have that all the matrix elements involved in Eqs. (13) and (14) are different of zero but the element M_{20}, in which $\Delta m=0$. Therefore, we have that for any frequency value (ω), the SHG coefficient is zero, i.e, $\chi^{(2)}_{2\omega}(\omega)=0$.

In the next section we present our calculations for the optical absorption and refractive index change in 2D-quantum dots. The several constants we have used are $\sigma_\nu=5\times10^{22}\ \mathrm{m}^{-3}$, $\hbar\Gamma_0=0.5$ meV, $\epsilon_0=8.85\times10^{-12}$ F/m, $q=1.6\times10^{-19}$ C, and $m^*=0.067\ m_0$, where m_0 is the free electron mass.

3. Results and discussion

As mentioned, the prototypical system under the study consists of a GaAs-based DSQD–QR. To help in the physical explanation of the THG results given below, Figs. 1–3 contain the calculated transition energies as well as the four dipole matrix elements entering Eq. (14). These quantities appear as function of the main input parameters of the model potential: the inverse square strength λ (Fig. 1), the magnetic field intensity (Fig. 2), and the parabolic potential amplitude (Fig. 3).

We observe, for instance, that the energy of transitions involving the first- and third-excited states in the system are decreasing functions of λ, whereas that corresponding to the transition