# Donor impurity-related nonlinear optical rectification in a two-dimensional quantum ring under magnetic field 

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## A R TICLE INFO

## Article history:

Received 24 May 2017
Received in revised form 5 August 2017
Accepted 11 August 2017
Available online 18 August 2017
Communicated by R. Wu

## Keywords:

Quantum ring
Donor impurity
Nonlinear optical rectification
Magnetic field
Semiconductors


#### Abstract

An investigation of the nonlinear optical rectification of a GaAs two-dimensional disc-shaped quantum ring with an off-center donor impurity under magnetic field has been performed by using a variational method in the effective mass approximation. The two-dimensional quantum ring was described by a pseudo-harmonic potential. The results are presented as functions of the incident photon energy for the different values of the impurity position and the magnetic field. It is found that the nonlinear optical rectification spectra are strongly affected by the position of the off-center impurity and the magnetic field.


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## 1. Introduction

The quantum rings (QRs) are semiconductor nanostructures that have attracted extensive theoretical and experimental investigations due to their unique electronic, magnetic and optical properties [1,2]. The QRs have found application in nanoelectronics, spintronics [3-5] and in quantum computational devices [6,7] because they present the Aharonov-Bohm effect [8-11]. Due to their potential technological applications and also to the intrinsic theoretical interest, the coupled QRs, or QR-quantum dots systems are the subject of some research as well (see $[12,13]$ and the references therein for a detailed discussion on single or coupled QRs).

In this work we investigate the effects of an off-center donor impurity on the optical rectification spectra of GaAs disc-shaped quantum ring (DSQR) under magnetic field. To describe the twodimensional quantum ring we used a pseudo-harmonic potential which is a combination of two potential profiles: an inverse square potential function and a parabolic potential that allows the description of the electron states in a quantum ring via analytical expressions in the absence of external lateral fields and impurity. For this reason it was used before by many groups like Chen et al. [14], Liu et al. [15] and by Duque et al. [16-18] who studied the dependence on the confinement potential and external fields of the photoionization cross section, the optical absorption coeffi-

[^0]http://dx.doi.org/10.1016/j.physleta.2017.08.024 0375-9601/© 2017 Elsevier B.V. All rights reserved.
cient, the variation of the refraction index and the third harmonic generation coefficient in this QR structures.

The effect of on-center impurity on the $Q R$ optical properties, using the potential we have chosen here, was addressed before by Chen et al. [14] and Duque et al. [16]. In our recent paper [19] we proved that off-center impurities significantly modify the electronic and optical properties of the structure, leading to new, characteristic effects. Particularly, in their presence, the rotational symmetry of the ring is destroyed, allowing obtaining an optical rectification spectrum. For this reason in present study we have taken three off-center positions of the impurity and we put in evidence the crucial role played by the impurity position on the optical rectification spectra calculated at different values of the magnetic field.

The outline of the paper is as follows. In Section 2 we describe the theoretical framework. The numerical results on the electronic properties and the nonlinear optical rectification spectra are presented and discussed in Section 3. A brief summary is given in Section 4.

## 2. Theory

The Hamiltonian of a two-dimensional disc-shaped quantum ring (DSQR) placed in the $(x, y)$ plane under a magnetic field can be written in the effective mass approximation as:
$H_{0}=\frac{1}{2 m^{*}}(\vec{p}+e \vec{A})^{2}+V(r)$
where $m^{*}$ is the effective mass of the electron, $e$ is the absolute value of the electron charge, $\vec{p}=-i \hbar \nabla=m^{*} \vec{r}-e \vec{A}(t)$ is the conjugate momentum of the position vector $\vec{r}$ of the electron [20], $\vec{A}$ is the potential vector of the magnetic field of intensity $\vec{B}$ applied perpendicular to the ring plane and $V(r)$ is the pseudo-harmonic confining potential of the quantum ring that combines an inverse square potential function with a parabolic function
$V(r)=\frac{\hbar^{2}}{2 m^{*}} \frac{\lambda^{2}}{r^{2}}+\frac{1}{2} m^{*} \omega_{0}^{2} r^{2}$.
Here $\lambda$ is a dimensionless parameter that characterizes the strength of the inverse square potential and $\omega_{0}$ represents the confinement frequency of the parabolic potential.

Using polar coordinates $(r, \varphi)$ and the Coulomb gauge $\vec{A}=$ ( $0, \mathrm{Br} / 2$ ) the Hamiltonian $H_{0}$ takes the form [14-18]:

$$
\begin{align*}
H_{0}= & -\frac{\hbar^{2}}{2 m^{*}}\left(\frac{\partial^{2}}{\partial r^{2}}+\frac{1}{r} \frac{\partial}{\partial r}+\frac{1}{r^{2}} \frac{\partial^{2}}{\partial \varphi^{2}}\right) \\
& +\frac{\hbar^{2}}{2 m^{*}} \frac{\lambda^{2}}{r^{2}}+\frac{1}{2} m^{*} \Omega^{2} r^{2}+\frac{\omega_{c}}{2} L_{z} \tag{3}
\end{align*}
$$

where $\Omega=\sqrt{\omega_{0}^{2}+\left(\frac{\omega_{c}}{2}\right)^{2}}$ is the total confinement frequency in magnetic field and $\omega_{c}=\frac{e B}{m^{*}}$ is the cyclotron frequency. $L_{z}$ is the orbital angular momentum operator along the $z$-direction. The solutions of the corresponding Schrödinger equation can be exactly described via analytical expressions [15-18] as:
$\psi_{n m}^{0}(r, \varphi)=N_{n m} \frac{\chi_{n m}(r)}{\sqrt{r}} e^{i m \varphi}$
where $N_{n m}$ is a normalization constant and $m=0, \pm 1, \pm 2 \ldots$ is the magnetic quantum number. The angular part of the function (4) is an eigenstate of the $L_{z}$ operator corresponding to the eigenvalue $m \hbar$. The radial function $\chi_{n m}(r)$ is [15-18]:
$\chi_{n m}(r)=r^{t_{m}} e^{-r^{2} / 2 \eta^{2}} L_{n}^{\left(t_{m}+1 / 2\right)}\left(r^{2} / \eta^{2}\right)$
where $\eta=\sqrt{\hbar / m^{*} \Omega}, t_{m}=1 / 2+\sqrt{\lambda^{2}+m^{2}}, n=0,1,2 \ldots$ and $L_{n}^{\left(t_{m}+1 / 2\right)}$ is the generalized Laguerre polynomial of order $n$.

The eigenvalues of the Hamiltonian from Eq. (3) have the following expression:
$E_{n, m}^{0}=\left(2 n+1+\sqrt{\lambda^{2}+m^{2}}\right) \hbar \Omega+m \hbar \omega_{c} / 2$.
In the presence of a donor impurity the Hamiltonian of the quantum system becomes:
$H=H_{0}-\frac{-e^{2}}{4 \pi \varepsilon_{0} \varepsilon_{r}\left|\vec{r}-\vec{r}_{\text {imp }}\right|}$
where $\varepsilon_{0}$ is the vacuum dielectric permittivity, $\varepsilon_{r}$ is the relative dielectric permittivity of the dot material and $\vec{r}_{i m p}=\left(x_{i m p}, 0\right)$ is the impurity position.

To calculate the eigenfunctions of the Hamiltonian from Eq. (7) we expanded them in the complete set of orthonormal wavefunctions $\psi_{n m}^{0}$ :
$\Psi_{i}(r, \varphi)=\sum_{n, m} a_{n, m}^{i} \psi_{n m}^{0}(r, \varphi)$
and the problem is reduced to solving a set of coupled equations for the coefficients $a_{n, m}^{i}$. In this linear variational calculation, a sufficient number of basis functions have been considered in order to obtain the desired convergence results. For each value of $B$, we organized 44 initial wavefunctions $\psi_{n m}^{0}$ with quantum numbers $n=0,1,2,3$ and $|m| \leq 5$ in the order of increasing energy and the first 21 states were used to diagonalize the Hamiltonian. This
choice ensures the convergence of the energy levels with an accuracy less than 0.4 meV .

Among the optical properties of the quantum ring system under magnetic field we have chosen to investigate here the nonlinear optical rectification. For a transition between two levels $E_{i}=\hbar \omega_{i}$ and $E_{j}=\hbar \omega_{j}$, the nonlinear optical rectification (NOR), calculated within the compact density-matrix formalism under steady state conditions and in the extended rotating wave approximation for coherent laser-matter interaction of asymmetric quantum structures, can be written as [21]:

$$
\begin{align*}
\chi_{0}^{i j}(\omega)= & \frac{2\left|\rho_{j}-\rho_{i}\right| \mu_{i j}^{2}\left|\mu_{j j}-\mu_{i i}\right| e^{3} T_{1} T_{2}}{\varepsilon_{0} \hbar^{2}} \\
& \times \frac{\left(J_{0}\left(\frac{\left|\mu_{j j}-\mu_{i i}\right| e E_{0}}{\hbar \omega}\right)+J_{2}\left(\frac{\left|\mu_{j j}-\mu_{i j}\right| e E_{0}}{\hbar \omega}\right)\right)^{2}}{1+T_{2}^{2}\left(\omega-\omega_{j i}\right)^{2}+\bar{\mu}_{i j}^{2} E_{0}^{2} T_{1} T_{2} / \hbar^{2}}, \tag{9}
\end{align*}
$$

where $\omega_{j i}=\omega_{j}-\omega_{i}$ and

$$
\begin{align*}
\bar{\mu}_{i j}= & e \mu_{i j}\left(J_{0}\left(\frac{\left|\mu_{j j}-\mu_{i i}\right| e E_{0}}{\hbar \omega}\right)\right. \\
& \left.+J_{2}\left(\frac{\left|\mu_{j j}-\mu_{i i}\right| e E_{0}}{\hbar \omega}\right)\right) \tag{10}
\end{align*}
$$

In Eqs. (9)-(10) $J_{0}, J_{2}$ are the ordinary Bessel functions of order 0 and $2, T_{1}$ is the population decay time and $T_{2}$ is the dephasing time. $E_{0}$ is the amplitude of the electric field $E(t)=E_{0} \cos (\omega t)$ related to the incident intensity $I_{0}$ of the probe field by $I_{0}=\frac{\varepsilon_{0} \subset n_{r} E_{0}^{2}}{2}$, where $n_{r}$ is the refractive index and $c$ the vacuum speed of light. The electric dipole matrix elements read as:
$\mu_{i j}=\left\langle\Psi_{i}(r, \varphi)\right| r \cos \varphi\left|\Psi_{j}(r, \varphi)\right\rangle$,
for a polarization of the incident radiation along the $x$-axis.
Using the density of states in the subband $E_{i}$ of the DSQR
$d_{i}(E)=g_{i} /\left(\pi \hbar S_{r}\right) \sqrt{2 m^{*}}\left(E-E_{i}\right)^{-1 / 2} \Theta\left(E-E_{i}\right)$
where $g_{i}$ is the degeneracy of the state $i$ (spin excluded), $S_{r}=$ $\pi\left(R_{2}^{2}-R_{1}^{2}\right)$ is the cross-sectional transverse area of the ring having $R_{1}, R_{2}$ as inner and outer radiuses and $\Theta$ is the Heaviside function, the density of the electrons at thermal equilibrium in the subband $E_{i}$ can be expressed as [22]:
$\rho_{i}=\frac{g_{i}}{\pi \hbar S_{r}} \sqrt{2 m^{*}} \int_{E_{i}}^{\infty} \frac{1}{\sqrt{E-E_{i}}}\left[1+\exp \left(\frac{E-E_{F}}{k_{B} T}\right)\right]^{-1} d E$.
Here $E_{F}$ is the Fermi level, $T$ is the absolute temperature and $k_{B}$ is the Boltzmann constant. The Fermi level $E_{F}$ at a given temperature may be determined from the charge neutrality condition:
$N=\sum_{i} \rho_{i}$
where the index $i=1,11$. The calculations are done in the low temperature limit, i.e. we take $T=4 \mathrm{~K}$ and N used in calculations is $3.2 \times 10^{23} \mathrm{~m}^{-3}$.

As the NOR coefficient of the low-dimensional systems is closely related to the asymmetries of the confinement potential, the NOR coefficient is zero for symmetric systems where the intrinsic dipole moments are zero. Therefore we emphasize that only the presence of an off-center impurity in the considered DSQR system allows to obtain a nonzero NOR coefficient.

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