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Optical coefficients in a semiconductor quantum ring: Electric field and donor impurity effects

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ABSTRACT

The electron states in a two-dimensional quantum dot ring are calculated in the presence of a donor impurity atom under the effective mass and parabolic band approximations. The effect of an externally applied electric field is also taken into account. The wavefunctions are obtained via the exact diagonalization of the problem Hamiltonian using a 2D expansion within the adiabatic approximation. The impurity-related optical response is analyzed via the optical absorption, relative refractive index change and the second harmonics generation. The dependencies of the electron states and these optical coefficients with the changes in the configuration of the quantum ring system are discussed in detail.

1. Introduction

Quasi-zero-dimensional semiconductor nanostructures such as quantum dots (QDs) and quantum rings (QRs) are subjects of great current interest regarding their prospective applications in the design and production of optoelectronic devices [1–5]. They have been obtained with the use of modern crystal-growth techniques. To mention just a few of those growing methods we can refer here to the so-called self-assembly procedure (see, for instance, reference [6–8]), the chemical liquid phase synthesis -in the case of nanocrystals made of ionically bonded materials- and the plasma-assisted processes for covalently bonded structures [9]. The possibility of fabricating artificial molecules consisting of coupled QDs [10] or QRs reveals as an attractive option for developing quantum information processing [11] and terahertz device production [12].

Atomic force microscopy imaging has revealed that the dimensions of anisotropic self-assembled InAs/GaAs QRs show values of the radius in the range of 11.5 nm and height in the range of 1.6 nm [13]. From the theoretical point of view a three-dimensional finite-element calculation based on elasticity theory has been applied to determine the relaxation of the cleaved surface of the modeled QR [14]. The single-particle Schrödinger equations were solved within the adiabatic approximation thus allowing to uncouple the radial and the in-growth-direction motions in the heterostructure. As a consequence, the phenomenon becomes essentially characterized by the radial carrier motion due to the fact that only one axial state appears confined along the growth direction. Multiple coupled 2D-like quantum rings with vertical size running in the range between 2 and 5 nm and values of the radii in the range of hundreds of nanometers have been reported as well [15–18].

Szafran et al. [19] performed a variational study of the evolution of lower energy exciton spectrum in a quantum ring described in the form of a 2D circular quantum dot with a repulsive core. They have shown that the radiative transition probability (TP) from the ground exciton state becomes largely enhanced by the effect of the repulsive core. At the same time the TP related to transitions starting at excited states significantly reduces. Besides, with the use

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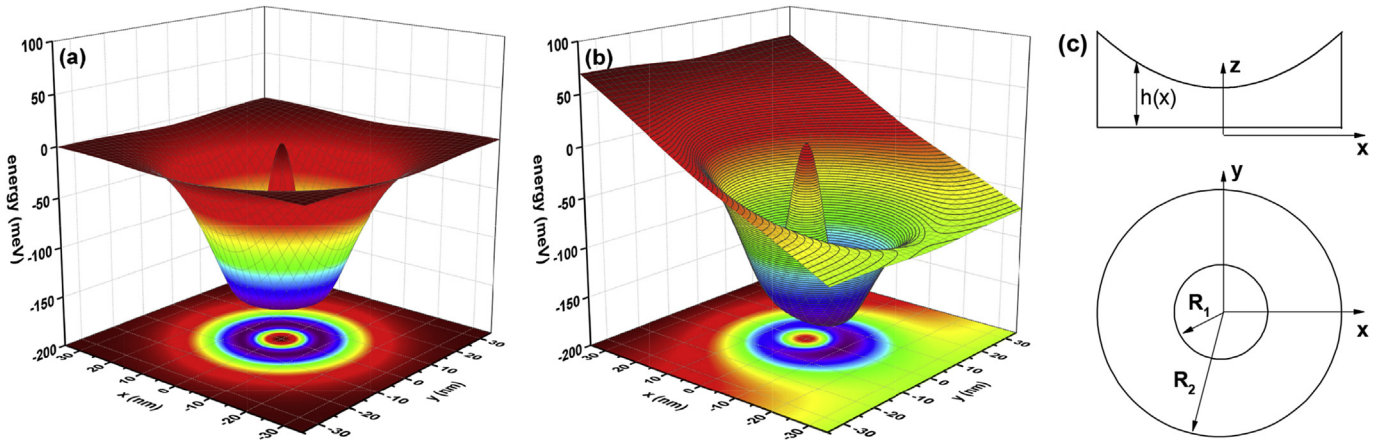

Fig. 1. Radial confinement potential plus electric field effect [$V_1(\rho) + |e|\,F\,x$ from Eqs. (2) and (3)] in a GaAs-Al_xGa_{1-x} As quantum ring as a function of the in-plane coordinates. Results are for two setups of (k,F): (1.0,0) (a) and (1.0,20 kV/cm) (b). The inner radius is set at 6 nm and the outer radius is taken equal to 18 nm. The quantum ring is centered at the center of the squared regions. In (c) are presented the xz and xy projections of the real structure.

of exact diagonalization techniques within the effective mass approximation, Szafran et al. [20] investigated a 2D N-electron system in a 2DQD coupled laterally to a surrounding QR. The authors considered the presence of an external magnetic field. Their results show that the distribution of electrons between the dot and the ring is affected by the relative strength of the confining potential energies of the dot and the ring as well as by the magnetic field strength, which induces electron transitions between QD and QR regions.

Liu et al. [21] put forward a model for describing the potential energy function in a 2DQR making use of a combination of a parabolic and inverse square functions. Within such approach it is possible to obtain analytical expressions for the electron states and energies, incorporating the effects of an externally applied electric field. The inclusion of a Coulombic center in the form of an ionized impurity atom in a so-described system was treated via perturbation theory in Ref. [22], where we also presented the impurity-related optical response. The problem of hydrogenic impurity (HI) states in a QR structure appears treated in a number of previous reports [23–27]. In particular, the effects of an externally applied DC electric field on the HI states in a QR were investigated in Ref. [28].

Motivated by the above mentioned works we aim at addressing the problem of the donor HI states plus a DC field in a GaAs-based 3-dimensional QR with fixed and/or variable height. For that purpose we implement a diagonalization approach to obtain the energy levels and wavefunctions. With the use of these states, we calculate the coefficients of the linear optical absorption (OA), the linear relative refractive index change (RRIC) and the second harmonics generation (SHG) associated with electron-impurity interstate transitions. The organization of the work is as follows. In Section 2 we describe the theoretical framework. Section 3 is dedicated to the discussion of the obtained results, and our conclusions are given in Section 4.

2. Theoretical framework

Here we shall consider the motion of conduction band electrons in the QR configuration that arises from the combination of a three-dimensional disc-shaped quantum dot (DSQD) with the effect of four distinct sources of potential energy: a radial confinement potential associated with radial-variations of the Aluminum concentration, an infinite potential in the top and bottom faces of the ring, the Coulombic attraction due to an ionized donor atom, and a DC-electric field [in Cartesian coordinates $(+F, 0, 0)$,].

The Hamiltonian of the system, within the framework of the effective mass approximation, is given by:

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V_1(\rho) + V_2(z) + \Big|e\Big|Fx - \frac{e^2}{\varepsilon\rho}, \tag{1}$$

or in the equivalent form

$$H = -\frac{\hbar^2}{2m^*}\nabla_\rho^2 - \frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + V_1(\rho) + V_2(z;x,y) + \Big|e\Big|Fx - \frac{e^2}{\varepsilon\rho}. \tag{2}$$

The quantities $|e|$ and m^* are the absolute value of the electron charge and the electron effective mass, respectively. ∇^2 and ∇_ρ^2 are the three-dimensional and in-plane Laplacian operators, respectively, $\overrightarrow{\rho} = (x, y)$ is the in-plane vector-position for the electron, and ρ is the electron-impurity distance (here we consider that the impurity is placed at the center of the ring system). The fourth term in the right-hand side of Eq. (2) —$V_2(z;x,y)$— means that the z-dependent confinement potential depends of the in-plane coordinates (x,y) (in this work this dependence is associated to the variations of the height of the ring). $V_2(z;x,y)$ is zero for $0 \le z \le h(x,y)$ and infinite for $z < 0$ and $z > h(x,y)$, where h is the height of the QR. The radial confinement potential is given by [19].

$$V_1(\rho) = -V_0\left[e^{-(\rho/R_2)^2} - ke^{-(\rho/R_1)^2}\right]. \tag{3}$$

In this expression R_1 and R_2 are the inner and outer radii of the QR, respectively, k —a dimensionless real-parameter— characterizes the strength of the repulsive potential at the core of the ring. The energy V_0 is equal to the barrier potential for electrons in GaAs surrounded by a Ga_{1-x} Al_xAs material ($V_e = Q\,\Delta E_g$, where Q is the band-offset and ΔE_g is the gap difference between the Ga_{1-x} Al_xAs and GaAs materials; Here we take $Q = 0.6$ and $\Delta E_g = 380$ meV, which corresponds to $x = 0.3$ for the Aluminum concentration).

Fig. 1 shows the shape of the potential energy profile with and without applied electric field, considering a radial confinement with $k = 1$.

Even, the problem with zero electric field and no impurity does not have analytical solutions. The inclusion of a nonzero electric field and/or the presence of a Coulombic term in the potential include new complications in order to find the eigenvalues and eigenfunctions of the Hamiltonian in Eq. (1). To find the