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Optical properties of hydrogenic impurity in an inhomogeneous infinite spherical quantum dot

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A R T I C L E I N F O

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A B S T R A C T

In the present work, using the effective mass approximation, the Schrödinger equation of system is solved in terms of Whittaker functions. The linear and third-order nonlinear optical absorption coefficient (AC) as well as refractive index (RI) changes associated with two intersubbund transitions (1s–2p and 2p–3d) in the case of a GaAs inhomogeneous infinite spherical quantum dot are investigated at different inner radii of shell and shell thicknesses. Regarding this, the optical properties of hydrogenic system are studied by means of compact density approach and dipole approximation. The results show that the system under study is strongly affected by inner radius of shell and shell thickness changes. Also it was found that the transition between orbital with bigger *l* value shift to higher photon energy region.

1. Introduction

Confined quantum systems have attracted much attention in the recent years. With the development of semiconductor nano-technology, the interest in the quantum and optical study of confined systems has increased [1–3]. Confined systems include quantum wells, quantum wires, quantum rings, and quantum dots. Many researchers studied the electronic structure by changing the shape and the size of such systems that leads to the formation of the discrete energy eigenvalues and also a removal of a part of degeneracy in comparison with the corresponding bulk materials. Therefore, many authors have studied the quantum properties, for example ground and excited states' energy, binding energy and also probability density [4,5].

Optical properties of confined systems have the potential for devising applicable structures such as photo-detectors, quantum dot lasers, high-speed electro-optical modulators and light emitting diodes; thus many researchers have studied the optical properties such as the linear, nonlinear and total absorption coefficient and refractive index changes [6–26]. Different methods are employed to obtain these properties such as variational [4,5], exact solution [6,7], Quantum Generic Algorithm [8] and perturbation theory [9].

Another newly found classification is the single-layered and multi-layered quantum systems. Much of the previous research is restricted to single-layered quantum dots and quantum anti-dots within different potential shapes and dimensions; however, several researches focused on multi-layered quantum systems [27–30].

In Ref. [6], the authors have obtained the exact solutions of Schrödinger equation for the electron in Coulomb field of hydrogenic donor impurity within the effective masses approximation and dielectric continuum model for the spherical quantum dot CdS/SiO_2 and anti-dot $ZnS/Cd_xZn_{1-x}S$. The dependence of electron energy spectrum and its probability density on nano-system radius have been studied. Oscillator strengths of the quantum transition with hydrogenic donor impurity, for transitions from the ground state to allowed first two excited states, in two and three dimensions, with both finite and infinite potential energy barriers are investigated in Ref. [7]. From numerical calculation, the results show that, in particular, the oscillator strength corresponding to the transitions from the ground state to the second excited state, though insignificant for small antidot radii, becomes notably large and indeed comparable with that of the transitions to the first excited state for large enough antidot radii.

In Ref. [8], quantum and optical properties of one-electron quantum dot with and without an on-center hydrogenic impurity were investigated in the case of finite depth confining potential. The energy eigenvalues and the state functions of quantum dot were calculated by using a combination of QGA and Hartree Fock Roothan methods. The authors calculated the binding energy for the states s, p, d and f oscillator strengths, the linear and third-order nonlinear optical absorption coefficients as a function of the incident photon energy and the incident optical intensity for the s–p, p–d and d–f transitions. It was found that the existence of the impurity has great influence on the optical absorption spectra and the oscillator strengths. Also the calculations show that the magnitudes of the

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total absorption coefficients of the spherical QD increase for transitions between higher states.

In this paper, all energy values are measured in unit of meV, and distances are expressed in nm. It is easy to show that the effective Bohr radius and the effective Rydberg energy can be obtained as $a_0^* = 4\pi\varepsilon\hbar^2/(m^* e^2)$ and $Ry^* = m^* e^4/2\hbar^2(4\pi\varepsilon)^2$ respectively. In the case of GaAs media the values of effective electron mass (m^*) and permittivity of media (ε) are $0.067m_e$ and $13.18\varepsilon_0$ respectively, where m_e and ε_0 are respectively the free electron mass and the permittivity of free space. Thus the effective Rydberg is numerically $Ry^* = 5.2$ meV and the effective Bohr radius, $a_0^* = 10.4$ nm.

The rest of this paper is organized as follows: In Section 2, the time independent Schrödinger equation with most general solutions and also the relations for AC and RI are presented. Numerical results and a brief summary are presented in Sections 3 and 4 respectively.

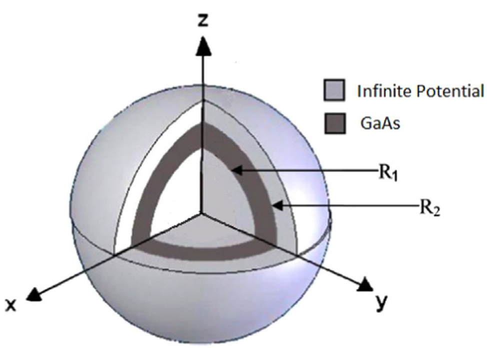

Fig. 1. A schematic view of confined system.

2. Theory and formulation

2.1. Energy eigenvalues and wave functions

Let us consider a hydrogenic impurity located in the infinite confining potential as designed in Fig. 1. The three dimensional time independent Hamiltonian of the confined system can be written as

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(r) - \frac{e^2}{4\pi\varepsilon r} \tag{1}$$

where

$$V(r) = \begin{cases} 0, & R_1 \le r \le R_2 \\ \infty & \text{elsewhere} \end{cases} \tag{2}$$

and $V(r)$ is the confining potential, R_1 and R_2 are the inner and outer radii of shell of hydrogenic impurity respectively; therefore $(R_2 - R_1)$ is the thickness of shell.

Schrödinger equation of this system in spherical coordinate is given by

$$-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Psi + \left(V(r) - \frac{e^2}{4\pi\varepsilon r}\right)\Psi = E\Psi \tag{3}$$

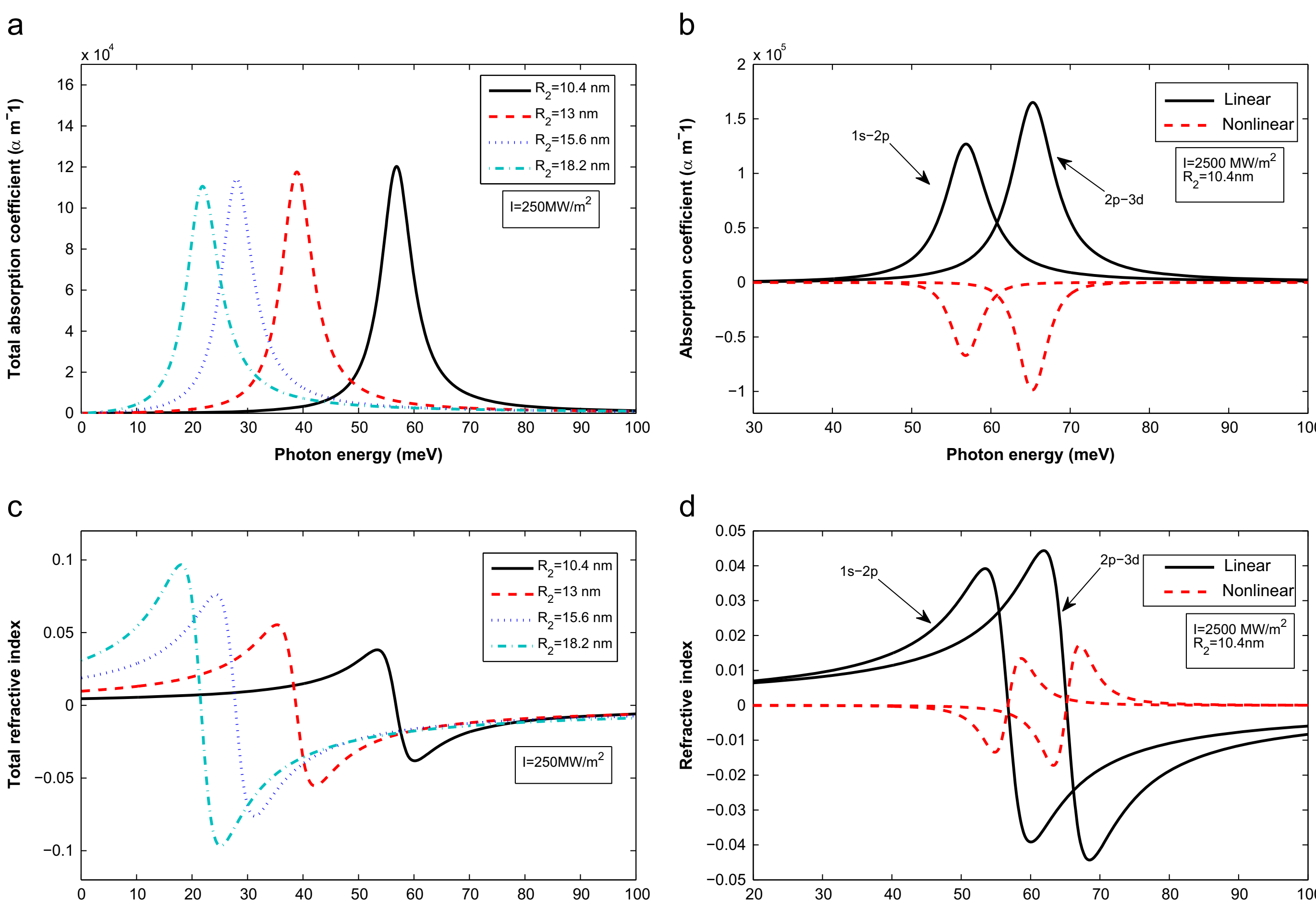

Fig. 2. Total AC for several dot radii (a), linear and nonlinear ACs for two transitions (b), total RI for several dot radii (c) and linear and nonlinear RIs for two transitions (d) as the function of incident photon energy.