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Optical absorption of a hydrogenic impurity in a disc-shaped quantum dot

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ABSTRACT

Using the perturbation method and the effective-mass approximation, we studied a hydrogenic impurity confined in a disc-shaped quantum dot with a parabolic potential in the presence of an electric field. Both the electric field and the confinement effects on the transition energy and the oscillator strength were investigated. Based on the computed energies and wave functions, the linear, the third-order nonlinear and the total optical absorption coefficients were also calculated. The results show that the optical absorption coefficients obtained in a disc-shaped parabolic QD can reach the magnitude of 10^4/cm, which is 1–2 orders of magnitude higher than that in the case of a spherical parabolic QD. We found that the transition energy, the oscillator strength, the linear, the third-order nonlinear and the total optical absorptions of the hydrogenic impurity in a disc-shaped QD dependent strongly on the confinement strength, and the applied electric field intensity.

1. Introduction

Understanding the impurity states in the confined systems is an important problem in semiconductor physics. Impurities in low-dimensional structures are introduced in order to modify the conduction and optical properties. The positively charged impurity with one electron can form the neutral donor in low-dimensional structures. Bastard [1,2] was the first to deal with the problem of the binding energy of the hydrogenic impurity in a quantum well. Lee and Spector [3] calculated firstly the binding energy of a hydrogenic impurity in quantum wires. Zhu et al. [4] studied the binding energy of a hydrogenic impurity in a spherical quantum dot (QD).

Modern techniques, like self-organized growth or molecular beam epitaxy, allow scientists to fabricate QDs with controllable size, shape, and other properties. It is expected that the fabrication of semiconductors with zero dimensions will show exotic electronic behavior such as the observation of discrete electronic states in GaAlAs/GaAs nanostructures and the photoluminescence of overgrown GaAlAs/GaAs QDs due the electronic confinement. The main features of QDs to be considered are their geometrical shape, size, and the confining potential. The electronic properties of a hydrogenic impurity in QDs have been investigated by many authors [5–10]. These features are useful for the development of optoelectronic devices with tunable emission or transmission properties and ultra-narrow spectral linewidths. In addition, external perturbations such as the application of an electric or magnetic field, can provide much valuable information about the hydrogenic impurity states. Therefore the energy spectrum of the systems can be varied substantially. Very recently, the electric field effect on the binding energy of impurity states in QDs has been investigated [11–14]. However, most of these studies were concerned with the ground-state electronic properties.

There is also an extensive interest in the optical phenomena based on intersubband transitions in semiconductor QDs. Due to the generally larger values of dipole matrix elements and the possibility of achieving the resonance conditions, both the linear and nonlinear optical processes in these structures are widely investigated [15–18]. In the optical absorption of quantum confined few-particle systems, the analysis of a hydrogenic impurity is inevitable because the confinement of quasiparticles in such structure leads to the enhancement of the oscillator strength of electron-impurity excitations. Meanwhile, the dependence of the optical transition energy on the confinement strength (or dot size) allows the tunability of the resonance frequency. Recently, optical absorption spectra associated with shallow hydrogenic impurities in a spherical QD have been investigated by Silva-Valencia and Porras-Montenegro [19]. However, to our knowledge, there are only few studies on the effects of electric fields for oscillator strength and nonlinear optical absorptions of a hydrogenic impurity in disc-shaped QDs [17,20].

Since QDs are created mainly by imposing a lateral confinement to electrons in a very narrow quantum well. QDs fabricated this way usually have the shape of a flat disk with lateral dimensions

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considerably exceeding their thickness. The energy of single-electron excitations across the disk exceeds other characteristic energies in the system, and the confined electrons can be considered as strictly two-dimensional. In most studies, a harmonic oscillator potential was used to describe the lateral confinement of electrons. Thus, it is interesting to investigate the electric and optical properties of a hydrogenic impurity in a disc-shaped QD with parabolic confinement potential in the presence of an electric field. In our present work, we will focus on studying the effects of an electric field and the confinement strength on the optical transition energy, the oscillator strength and the linear, the third-order nonlinear and the total optical absorptions of a hydrogenic impurity in a disc-shaped QD. From the consideration of device applications, engineering the electronic structure of materials by means of external field and confinement strength offers the possibility of tailoring the energy spectrum to produce desirable optical absorptions.

2. Theory

Within the framework of effective-mass approximation, the Hamiltonian of a hydrogenic impurity confined in a disc-shaped QD with a parabolic potential in the presence of an electric field can be written as

$$H=\frac{p^2}{2m_e}+\frac{1}{2}m_e\omega_0^2r^2+|e|\vec{F}\cdot\vec{r}-\frac{e^2}{\epsilon r}, \tag{1}$$

where $\vec{r}(\vec{p})$ is the position vector (the momentum vector) of the electron originating from the center of the dot, m_e is the effective mass of an electron, ω_0 measures the strength of the confinement and ϵ is the dielectric constant. The external electric field is applied in the x direction. The Hamiltonian can be rewritten as

$$H=H_0+H' \tag{2}$$

with

$$H_0=\frac{p_x^2}{2m_e}+\frac{1}{2}m_e\omega_0^2(x+\beta)^2+\frac{p_y^2}{2m_e}+\frac{1}{2}m_e\omega_0^2y^2-\frac{1}{2}|e|F\beta, \tag{3}$$

and

$$H'=-\frac{e^2}{\epsilon r}, \tag{4}$$

where $\beta=|e|F/(m_e\omega_0^2)$. In the regime of strong confinement, H' is assumed the perturbation term. The perturbation methodology has been used to treat the two-electron systems of QDs in the regime of strong confinement [21,22].

The eigenfunctions of the low-lying states of a hydrogenic impurity confined by a disc-shaped QD with a parabolic potential in the presence of an electric field and a magnetic field without the Coulombic interaction are given by

$$\Psi_{n_xn_y}(x,y)=\phi_{n_x}(x+\beta)\phi_{n_y}(y),\quad n_x,n_y=0,1,\ldots, \tag{5}$$

where

$$\phi_n(i)=N_n\exp(-\alpha^2i^2/2)H_n(\alpha i), \tag{6}$$

and

$$\alpha=\sqrt{m_e\omega_0/\hbar},\quad i=x,y. \tag{7}$$

Here $N_n=\left[\frac{\alpha}{\sqrt{\pi}2^nn!}\right]^{1/2}$ is the normalization constant, $H(\alpha i)$ is the Hermite polynomial, and $\phi_n(i)$ is the normalized wave function of one-dimensional oscillator. Introducing the polar coordinates

$$x=r\cos\theta,\quad y=r\sin\theta, \tag{8}$$

then we can obtain the wave functions of the three lowest states in polar coordinates, respectively,

$$\Psi_{00}(r,\theta)=\frac{\alpha}{\sqrt{\pi}}\exp(-\alpha^2r^2/2-\alpha^2\beta r\cos\theta-\alpha^2\beta^2/2), \tag{9}$$

$$\Psi_{01}(r,\theta)=\sqrt{\frac{2}{\pi}}\alpha^2r\sin\theta\exp(-\alpha^2r^2/2-\alpha^2\beta r\cos\theta-\alpha^2\beta^2/2), \tag{10}$$

and

$$\Psi_{10}(r,\theta)=\sqrt{\frac{2}{\pi}}\alpha^2(r\cos\theta+\beta)\exp(-\alpha^2r^2/2-\alpha^2\beta r\cos\theta-\alpha^2\beta^2/2), \tag{11}$$

where $\Psi_{00}(r,\theta)$ is the wave function of the ground state $(n_x=0,n_y=0)$, $\Psi_{01}(r,\theta)$ and $\Psi_{10}(r,\theta)$ are the wave functions of the first excited states with twofold degeneracy. The matrix elements of the Coulomb potential are given by

$$H'_{ij}=-\langle\Psi_{n'_xn'_y}|H'|\Psi_{n_xn_y}\rangle=-\frac{e^2}{\epsilon}\left\langle\Psi_{n'_xn'_y}\left|\frac{1}{r}\right|\Psi_{n_xn_y}\right\rangle, \tag{12}$$

where i and j are the suffixes of the matrix element about H'.

The oscillator strength is a very important physical quantity in the study of the optical properties which are related to the electronic dipole-allowed transitions. Generally, the oscillator strength P_{fi} is defined as

$$P_{fi}=\frac{2m_e}{\hbar^2}E_{fi}|M_{fi}|^2, \tag{13}$$

where $E_{fi}=E_f-E_i$ denotes difference of the energy between lower and upper levels, and $M_{fi}=e\langle\Psi_i|x|\Psi_f\rangle$ is the electric dipole moment of the transition from the Ψ_i state to the Ψ_f state. The oscillator strength can offer additional information on the fine structure and selection rules of the optical absorption [23]. Because the electric dipole moment of the transition from the Ψ_{00} state to the Ψ_{01} state is zero, in this work, we restrict our study to the transition between the Ψ_{00} and Ψ_{10} states.

The optical absorption calculation is based on the Fermi's golden rule and the compact density-matrix approach, for which the optical absorption coefficient is given by [24]

$$\alpha(\upsilon,I)=\alpha^{(1)}(\upsilon)+\alpha^{(3)}(\upsilon,I), \tag{14}$$

where

$$\alpha^{(1)}(\upsilon)=\frac{4\pi\beta_{FS}\sigma_s}{n_re^2}h\upsilon|M_{fi}|^2\delta(E_{fi}-h\upsilon), \tag{15}$$

and

$$\alpha^{(3)}(\upsilon,I)=-\frac{32\pi^2\beta_{FS}^2\sigma_sI}{n_r^2e^4\hbar\Gamma_{ff}}h\upsilon|M_{fi}|^4\delta^2(E_{fi}-h\upsilon)\times\left\{1-\frac{|M_{ff}-M_{ii}|^2}{4|M_{fi}|^2}\frac{[(h\upsilon-E_{fi})^2-(\hbar\Gamma_{fi})^2+2E_{fi}(E_{fi}-h\upsilon)]}{E_{fi}^2+(\hbar\Gamma_{fi})^2}\right\}, \tag{16}$$

are the linear and the third-order nonlinear optical absorption coefficients, respectively. n_r is the refractive index of the semiconductor and it is taken as 3.2. e is the electronic charge of an electron, σ_s is the electron density in the QD, $\beta_{FS}=e^2/(4\pi\epsilon_0\hbar c)$ is the fine structure constant, I is the incident optical intensity, and $h\upsilon$ is the photon energy. The first and the second terms of Eq. (14) are the linear and the third-order nonlinear optical absorption coefficients $\alpha^{(1)}(\upsilon)$ and $\alpha^{(3)}(\upsilon,I)$, respectively. The δ function in Eqs. (15) and (16) are replaced by a narrow Lorentzian by means of

$$\delta(E_{fi}-h\upsilon)=\frac{\hbar\Gamma_{fi}}{\pi[(h\upsilon-E_{fi})^2+(\hbar\Gamma_{fi})^2]}. \tag{17}$$

Here Γ is the phenomenological operator. Nondiagonal matrix element Γ_{fi} $(f\neq i)$ of operator Γ, which is called as the relaxation rate