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The low-lying states and optical absorption properties of a hydrogenic impurity in a parabolic quantum dot modulation by applied electric field

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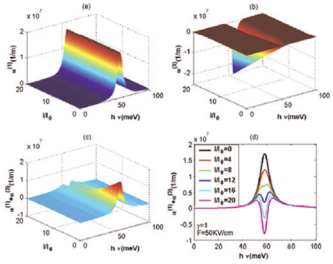
HIGHLIGHTS

- We investigated the low-lying states and optical absorption properties of a hydrogenic impurity using CI method.
- The low-lying states and optical absorption properties depend sensitively on the electric field and the confined potential.
- The magnitude of optical absorption coefficients in parabolic SQDs is high about 10^7/m.
- The blue-shift (red-shift) of the peak of optical ACs appears.

GRAPHICAL ABSTRACT

The low-lying states and optical absorption properties of hydrogenic impurity are investigated in parabolic quantum dots modulation by applied electric field using the configuration-integration method.



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ABSTRACT

Using the configuration-integration method, we investigated theoretically the low-lying states and optical absorption properties of a hydrogenic impurity in a parabolic quantum dot modulation by applied electric field. The low-lying states and optical absorption properties depend sensitively on the electric field F and the strength of the parabolic confinement $\hbar\omega_0$. We discuss the linear and third-order nonlinear optical absorption coefficients of the dot (i) with the impurity ion and (ii) without the impurity ion. In the first case, the increase of the parabolic confinement $\hbar\omega_0$ (or the electric field F) can induce the blueshift (or redshift) of the peak of the absorption coefficient. Also the optical intensity can induce the increase of the third-order nonlinear optical absorption coefficients to weaken and even bleach the total optical absorption coefficients. Similar behavior has also been observed in the second case, but there is no redshift of the peak positions of the absorption coefficient with the increase of the electric field F. Compared with the second case, it is easily seen that there are the blueshifts of the peak of the absorption coefficients, which can be used as a technical means for detecting impurities.

1. Introduction

There has been an increasing interest in the investigation of quantum dots (*QDs*) due to their intrinsic physical properties and technological applications in electronic devices [1–40]. Using these techniques such as etching and molecular beam epitaxy, quantum dot (*QD*) can be fabricated in different shapes, such as disk-like (cylindrical) shape and spherical shape [1]. So far, the spherical quantum dots (*SQDs*) have been formed from semiconductor nanocrystals embedded in either an insulating [2] or a

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semiconducting matrix [3]. In *SQDs*, the charge carriers (electrons and holes) are confined in all three dimensions [4–8]. The new, unusual properties of the low-dimensional nanometer-sized semiconductor give rise to a full quantum nature to these structures. *SQDs* are expected to exhibit enhanced optical nonlinearities and enhanced electro-optic effects [9].

The study of impurities in semiconductors has attracted much attention in recent years because of its potential applications in the optical devices. All semiconductor devices factually incorporate dopants as a crucial ingredient for their proper functioning. Thus an understanding of the nature of impurity states in semiconductor structures is one of the crucial problems in semiconductor physics. As is known, the impurities in semiconductors can affect the electrical, optical and transport properties [10,11]. Thus, impurities play an essential role in semiconductor devices. For example, the semiconductor structures with quantum confinement show interesting physical properties, which depend not only on the strength of parabolic confinement but also on the external electric field [10,12]. The study of hydrogenic impurity states in semiconductor nanostructures can date back to the early 1980s through the pioneering work of Bastard [13]. In spite of growing interest in the topic of impurity doping in nanocrystallites, most theoretical work carried out on the shallow donor impurity in *SQDs* employs variational approaches [14–20], alternatively, perturbation methods are limited to the strong confinement regime [21–23]. Recently, some new methods have been applied to solve these relevant problems above. Li [24] has calculated the electronic states of a hydrogenic donor impurity in low-dimensional semiconductor nanostructures in the framework of effective-mass envelope-function theory by using the plane wave method. Xie [25] and Zhu et al. [26] have investigated the binding energy of hydrogenic donor impurity in a parabolic quantum dot and in a rectangle spherical quantum dot using the method of numerical diagonalization, respectively. The topic for the various confined potential in the *QD* using potential morphing method (*PMM*) has been reported by Baskoutas et al. for investigating the low-lying state and optical properties [27,28]. However, the binding energy and nonlinear optical properties of the low-lying states of donor impurity with the external electric field were not taken into account by the above-mentioned authors but the authors of Refs. [23,28]. And most of the researches about this topic were carried out by the variational approaches [12,19].

In this work, we will investigate theoretically the low-lying states and optical absorption properties of a hydrogenic impurity in a parabolic *QD* modulation by the applied electric field. An attempt is to study the influence of the external electric field, and parabolic confinement strength on the low-lying states and optical absorption properties of a hydrogenic impurity in a parabolic *QD* using the configuration-integration methods (*CI*) [29]. Our numerical calculations are carried out for one of the typical semiconducting materials, GaAs. It is found that the low-lying states and optical absorption properties depend sensitively on the electric field F and the strength of the parabolic confinement $\hbar\omega_0$. We discuss the linear and third-order nonlinear optical absorption coefficients (*ACs*) of the dot (i) with the impurity ion and (ii) without the impurity ion. It is seen that the optical *ACs* obtained in parabolic *SQDs* can reach the magnitude of 10^7/m. In the first case, the increase of the parabolic confinement $\hbar\omega_0$ (or the electric field F) can induce the blueshift (or redshift) of the peak of the *ACs*. Also the optical intensity can induce the increase of the third-order nonlinear optical *ACs* to weaken and even bleach the total optical *ACs*. Similar behavior has also been observed in the second case, but there is no redshift of the peak positions of the *ACs* with the increase of the electric field F. Compared with the second case, it is shown that there are the blueshifts of the peak of the *ACs*, which can be used as a technical means for detecting impurities. In Section 2, the model and the method for our calculation are introduced in detail. In Section 3, the numerical analysis to our important analytical issues is reported. Finally, a brief summary is given in Section 4.

2. Model and method

Within the framework of effective-mass approximation, the Hamiltonian of a center hydrogenic donor confined by a spherical *QD* with a parabolic potential in the presence of electric field along the z-axis can be written by

$$H = \frac{\mathbf{p}^2}{2m_e^*} + V(r) - \gamma\frac{e_s^2}{\varepsilon\mathbf{r}} + q\mathbf{F}\cdot\mathbf{r}, \tag{1}$$

where the hydrogenic impurity is located at the center of the *QD*, e_s is the reduced charge of the electron, namely, $e_s = e/\sqrt{4\pi\varepsilon_0}$ and q is the absolute value of the electron charge e. $\mathbf{r}(\mathbf{p})$ 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 and $V(r)$ is the confining potential in the form of

$$V(r) = \frac{1}{2}m_e^*\omega_0^2 r^2, \tag{2}$$

where ω_0 is the strength of the confinement potential frequency. In our model, the Hamiltonian of single hydrogenic impurity in a spherical *QD* can be expressed as the sum of the original harmonic oscillator Hamiltonian term H_0, a Coulomb interaction term H_1 and a electric potential term H_2, i.e.,

$$H = H_0 + H_1 + H_2, \tag{3}$$

where

$$H_0 = \frac{\mathbf{p}^2}{2m_e^*} + \frac{1}{2}m_e^*\omega_0^2\mathbf{r}^2, \tag{4}$$

$$H_1 = -\gamma\frac{e_s^2}{\varepsilon\mathbf{r}}, \tag{5}$$

$$H_2 = q\mathbf{F}\cdot\mathbf{r}. \tag{6}$$

In order to obtain the eigenfunction and eigenenergy associated with the hydrogenic donor in a spherical *QD*, let us consider a linear function of the form

$$\Psi_m = \sum_j c_j\psi_j(r,\theta,\varphi), \tag{7}$$

where $\psi_j(r)$ is a *3D* harmonic oscillator state with the frequency ω_0 and an energy $(2n_j + l_j + 3/2)\hbar\omega_0$. The principal, orbital, and magnetic quantum numbers of $\psi_j(r,\theta,\varphi)$ are n_j, l_j, and m_j, respectively. In the presence of the electric field, only the magnetic quantum number is a good one. The summation in Eq. (7) includes only the terms with a fixed magnetic quantum numbers m (i.e., $m_1 = m_2 = \ldots = m$). Here, so j denotes the whole set quantum numbers n_j and l_j in brevity. Let $N_j = 2n_j + l_j$ and obviously the accuracy of solutions depends on the model spaces. The dimension of the model space is constrained by $0 \le N_j \le 30$. The matrix elements of H are then given by the following expressions:

$$\langle\Psi_m|H|\Psi_m\rangle = \sum_{i,j} c_i c_j\left\{\left[2n_j + l_j + 3/2\right]\hbar\omega_0\delta_{i,j} + u_{i,j}^{I} + u_{i,j}^{II}\right\}, \tag{8}$$

with