Solid State Communications 209-210 (2015) 27–32

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Polaronic effect on linear and nonlinear optical properties of spherical quantum dots under electric field

L. Shi, Z.W. Yan *

College of Sciences, Inner Mongolia Agricultural University, Hohhot 010018, PR China

ARTICLE INFO

Article history:
Received 7 November 2014
Accepted 27 February 2015
Communicated by A. Pinczuk
Available online 5 March 2015

Keywords:
A. Quantum dot
D. Electron–phonon interaction
D. Electric field

ABSTRACT

The polaronic effect on the linear and nonlinear optical properties of spherical quantum dots with a shallow hydrogenic impurity under electric field are studied, taking into account the interactions with both confined and surface optical phonons. In addition, the interaction between impurity and phonons has also been considered. Numerical results on typical $Zn_{1-x}Cd_xSe/ZnSe$ material show that the polaronic effect or electric field redshifts the peak positions of linear and nonlinear optical absorption coefficients and refractive index changes, but does not significantly affect the peak values of them. The polaronic effect is enhanced with the decreasing quantum dot radius or Zn concentrations. Additionally, it is found that the electric field has an important influence on the polaronic effect especially on the surface optical phonons.

1. Introduction

It is well known that optical properties such as optical absorption coefficients (ACs), refractive index changes (RICs) and oscillator strength have the potential for luminescent device research. Furthermore, there is no doubt that the zero-dimensional quantum dots (QDs) with well-controlled shape and size have became one of the hottest topics in the area of the condensed matter and materials physics due to their distinctive electronic and optical properties. Therefore, the optical properties of QDs have attracted the considerable attention in the experimental and theoretical studies in recent years [1–6].

Because electron–optical phonon interaction plays an important role in optical and electrical properties of QDs, it is still a interesting topic theoretically and experimentally. Compared with other nanostructures, the interaction between electron and phonon is more effectively in QDs because of its special structure. Besides the confined optical (CO) phonons, there exist surface optical (SO) phonons due to the difference in the dielectric constants of the materials inside and outside the structure, and it depends strongly on the QD shape and electric field [7]. There are many works about various forms: spherical QDs [8–10], cylindrical QDs [11–13], ellipsoidal QDs [14–16], and the polaronic effect has been studied in some works. It is found that the CO phonons play the most important role in the polaronic effect and the contribution from the SO phonons is either negligible or nonexistent. Unfortunately, in most of them the impurity–phonon interaction is either ignored or not discussed. In fact, the contribution from impurity–phonon interaction is very important and generally larger than that from electron–phonon interaction [17,18]. For these reasons, it can be said that the polaronic effect is important to the optical properties of QDs, and should be considered in the related works.

The applied electric field is quite useful as a powerful tool for studying the physical properties of semiconductors and modulating the properties of devices. The effect of applied electric field on the electronic states in QDs has been studied extensively by many authors in the past few years [17–21]. As known, the electric field induces both a polarization of the carrier distribution and an energy shift of the quantum states to introduce a considerable change in the energy spectra of carriers, and this property is very useful for optoelectronic devices. Because electric field has an important influence on the carrier distribution, the optical properties of QDs also depend on the electric field. There are some works about the optical properties of QDs under the influence of electric field [2,4,22], but the electron–phonon interaction is not considered. As a matter of fact, the electric field should have an important effect on the electron–phonon interaction. In particular, the SO phonon modes strongly depend on the electric field.

In the present work, taking the electron–phonon and impurity–phonon interactions into account, including CO and SO phonon modes, we investigate the influence of electric field on the linear and third-order nonlinear ACs and RICs of a spherical QD by using a variational approach. To come closer to the real situation, the electronic confinement is modeled by a finite potential well. This paper is organized in the following way. In Section 2, the ACs, RICs,

* Corresponding author. Tel./fax: +86 471 4309247.
E-mail address: zwyan101@126.com (Z.W. Yan).

http://dx.doi.org/10.1016/j.ssc.2015.02.023
0038-1098/

and the electron–phonon interaction are described. In Section 3, the general behavior of electron–phonon interaction, and the optical properties of the system under the influence of electric field are studied numerically. Finally, the conclusions are presented.

2. Theory and model

In the following, the interactions between electron and various phonon modes, the system Schrodinger equation and wave function, and ACs and RICs are introduced step by step.

2.1. Electron–phonon interaction

Let us consider a sphere of radius R embedded in a large medium. When an electron is inside ($r<R$) the QD, it will interact with the internal LO phonons, similar to the case in quantum well, we call it CO phonons. When the electron is close to the QD boundary ($r\approx R$), it will interact with the SO phonons. The classical Hamilton functions of CO and SO phonons can be written as follows:

$$H_{ph}^{\mathrm{CO}}=\sum_{lmn}\hbar\omega_{\mathrm{CO}}\left(a_{lmn}^{+}a_{lmn}+\frac{1}{2}\right), \tag{1}$$

$$H_{ph}^{\mathrm{SO}}=\sum_{lm}\hbar\omega_{\mathrm{SO},l}\left(a_{lm}^{+}a_{lm}+\frac{1}{2}\right), \tag{2}$$

where ω_{CO} and $\omega_{\mathrm{SO},l}$ are the eigenfrequencies of CO and SO phonons respectively. The Hamiltonian of both electron and impurity interact with CO and SO phonons can be written as [9,23]

$$H_{ep}^{\mathrm{CO}}=-\sum_{lmn}\beta_{lmn}^{\mathrm{CO}}\left\{\left[V_{lmn}^{\mathrm{CO}}(r)-V_{lmn}^{\mathrm{CO}}(r_0)\right]a_{lmn}+\mathrm{H.c.}\right\}, \tag{3}$$

$$H_{ep}^{\mathrm{SO}}=\begin{cases}-\sum_{lm}\beta_{lm}^{\mathrm{SO}}\left\{\left[V_{lm}^{\mathrm{SO}}(r)-V_{lm}^{\mathrm{SO}}(r_0)\right]a_{lm}+\mathrm{H.c.}\right\}, & r<R,\\ -\sum_{lm}\beta_{lm}^{\mathrm{SO}}\left[V_{lm}^{\mathrm{SO}}(r)a_{lm}+\mathrm{H.c.}\right], & r>R,\end{cases} \tag{4}$$

where

$$\beta_{lmn}^{\mathrm{CO}}=\left\{\frac{4\pi {e_s}^2}{R}\frac{\hbar\omega_{\mathrm{CO}}}{\mu_{\mathrm{ln}}^2 j_{l+1}^2(\mu_{\mathrm{ln}})}\left(\frac{1}{\varepsilon_{1\infty}}-\frac{1}{\varepsilon_{10}}\right)\right\}^{1/2}, \tag{5}$$

with

$$V_{lmn}^{\mathrm{CO}}(r)=j_l(k_{ln}r)Y_{lm}(\theta,\varphi), \tag{6}$$

and

$$\beta_{lm}^{\mathrm{SO}}=\frac{\varepsilon_{1\infty}\sqrt{l}}{l\varepsilon_{1\infty}+(l+1)\varepsilon_d}\omega_{\mathrm{CO}}\sqrt{\frac{2\pi e_s^2\hbar}{\omega_{\mathrm{SO},l}R}\left(\frac{1}{\varepsilon_{1\infty}}-\frac{1}{\varepsilon_{10}}\right)}, \tag{7}$$

with

$$\omega_{\mathrm{SO},l}^2=\frac{\left[\varepsilon_d+(\varepsilon_d+\varepsilon_{10})l\right]\varepsilon_{1\infty}}{\left[\varepsilon_d+(\varepsilon_d+\varepsilon_{1\infty})l\right]\varepsilon_{10}}\omega_{\mathrm{CO}}^2, \tag{8}$$

$$V_{lm}^{\mathrm{SO}}(r)=\begin{cases}(r/R)^l Y_{lm}(\theta,\varphi), & r<R\\ (R/r)^{l+1}Y_{lm}(\theta,\varphi), & r>R\end{cases}, \tag{9}$$

where j_l and n_l are the lth order spherical Bessel and Neumann functions respectively; $Y_{l,m}$ is spherical harmonics function; $k_{ln}=\mu_{ln}/R$, μ_{ln} is the nth root of j_l; $e_s=e/(4\pi\varepsilon_0)^{-1/2}$, and e is the absolute value of the electron charge, ε_0 is the permittivity of free space; $\varepsilon_{1\infty}$ ($\varepsilon_{2\infty}$) and ε_{10} (ε_{20}) are the high-frequency and static dielectric constants in dot (barrier) material respectively. The index $n=1, 2, \ldots$; $l=0, 1, 2, \ldots$; $m=0, \pm1, \pm2,\ldots, \pm l$ for the CO phonons, and $l=1, 2, \ldots$; $m=0, \pm1, \pm2,\ldots, \pm l$ for the SO phonons. In Eqs. (3) and (4), r and r_0 are the positions of electron and impurity (the center of the sphere is taken as the origin) respectively. In this paper, we assume that the impurity is at the center, i.e. $r_0=0$.

2.2. Variational procedure

Followed above, we can write the Hamiltonian of whole system in the presence of an external electric field along the z direction as

$$H=H_0+H_{ph}^{\mathrm{CO}}+H_{ph}^{\mathrm{SO}}+H_{ep}^{\mathrm{CO}}+H_{ep}^{\mathrm{SO}}, \tag{10}$$

$$H_0=\frac{p^2}{2m}-\frac{e_s^2}{\varepsilon r}+U(\vec{r})+|e|Fr\ \cos\ \theta, \tag{11}$$

$$U(\vec{r})=\begin{cases}0 & for \quad r\le R\\ U_0 & for \quad r>R\end{cases},\quad m=\begin{cases}m_1 & \text{for} \quad r<R\\ m_2 & \text{for} \quad r>R\end{cases},$$
$$\varepsilon=\begin{cases}\varepsilon_{1\infty} & \text{for} \quad r<R\\ (\varepsilon_{1\infty}+\varepsilon_{2\infty})/2 & \text{for} \quad r>R\end{cases}, \tag{12}$$

where m_1 (m_2) and $\varepsilon_{1\infty}$ ($\varepsilon_{2\infty}$) are the effective mass and high-frequency dielectric constant in dot (barrier) material respectively; $U(\vec{r})$ is the confinement potential of QDs; F is the strength of the electric field along the z direction; θ is the angle between the electronic position vector $\vec{r}$ and the electric field direction.

As is usually done for the bulk case, first it is necessary to eliminate the contribution to the total electron energy from the impurity–phonon interactions. This can be achieved by using a first unitary transformation to displace the equilibrium position of the ions

$$U=\exp\left\{\sum_{j=\mathrm{CO,SO}}\sum_{s}\left[\frac{\beta_s^j V_s^j(r_0)a_{js}^{+}+\mathrm{H.c.}}{\hbar\omega_j}\right]\right\}. \tag{13}$$

Here CO and SO denote the CO and SO phonons respectively. The index s is given by $n=1, 2, \ldots$; $l=0, 1, 2, \ldots$; $m=0, \pm1, \pm2, \ldots, \pm l$ for the CO phonons, and $l=1, 2, \ldots$; $m=0, \pm1, \pm2,\ldots, \pm l$ for the SO phonons. Then the Hamiltonian can be transformed into the following form:

$$H^{*}=U^{-1}HU=H_0+H_{ph}^{\mathrm{CO}}+H_{ph}^{\mathrm{SO}}+H'_{ep}\mathrm{CO}+H'_{ep}\mathrm{SO}+H_x, \tag{14}$$

where

$$H'_{ep}\mathrm{CO}=-\sum_{lmn}\beta_{lmn}^{\mathrm{CO}}\left[V_{lmn}^{\mathrm{CO}}(r)a_{lmn}+\mathrm{H.c.}\right], \tag{15}$$

$$H'_{ep}\mathrm{SO}=-\sum_{lm}\beta_{lm}^{\mathrm{SO}}\left[V_{lm}^{\mathrm{SO}}(r)a_{lm}+\mathrm{H.c.}\right]. \tag{16}$$

For convenience, we have dropped the nonphysical divergent term arising from the use of the point-charge model, the effect of above displacement on the lattice polarization leads to the following electron–impurity "exchange" interaction:

$$H_x=\sum_{j=\mathrm{CO,SO}}\sum_{s}\frac{|\beta_s^j|^2V_s^j(r_0)V_s^j(r)+\mathrm{H.c.}}{\hbar\omega_j}. \tag{17}$$

Within the adiabatic approximation, the effect of the electron–phonon interaction is to displace further the equilibrium positions of the ions. It can be achieved by the following unitary transformation:

$$U'=\exp\left\{\sum_{j=\mathrm{CO,SO}}\sum_{s}\left[f_{js}a_{js}^{+}+\mathrm{H.c.}\right]\right\}. \tag{18}$$

The parameters f_{js} are variational functions and will be determined by minimizing the expectation value of the bound polaron energy. The total wave function of the system is given by the product of