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The ground-state transition probability of impurity bound polaron in quantum rod

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ABSTRACT

We using a variational method of Pekar type to study the ground-state transition probability of impurity bound polaron with strong electron–LO-phonon coupling in a quantum rod (QR). Quantum transition is happened in the low dimensional quantum system due to the electron–phonon interaction and the impact of temperature. That is the polaron transit from the ground-state to the first-excited state after absorbing a LO-phonon. We find the ground-state transition probability of impurity bound polaron enlarger with increasing the transverse and longitudinal confinement lengths of QR and changes small with enhancing the ground-state energy of impurity bound polaron. And the ground-state transition probability of bound polaron is an increasing function of the electron–phonon coupling constant.

1. Introduction

In the last decade, with the developments in epitaxial technology, such as molecular-beam epitaxy and nanothography, it becomes possible to produce these systems, which are typified by hetero-interfaces between the different semiconductors. Consequently optical properties of low-dimensional semiconductor systems have received considerable research interest both experimentally and theoretically. In practice, in a quantum rod (RD) system, the electron–phonon interactions are enhanced by the geometric confinement. Therefore, some works on the electron–phonon interaction in low dimensional quantum systems have been studied. Landau and Pekar [1–4] researched the physical properties of polarons, in the today's terminology these first studies were all devoted to the strong-coupling theory. An improved model of electron–phonon interaction for longitudinal-optical phonons in layered semiconductor quantum wells was studied by Wendler [5]. Xiao et al. [6] calculated the coulomb bound potential quantum rod qubit, which is strongly coupled to LO-phonon, by using the variational method of Pekar type. Verzelen et al. [7] investigated the polaron lifetime and energy relaxation in semiconductor quantum dots. The results show that a harmonicity driven instability of optical phonons leads in semiconductor quantum dots to a decay of polaron states which otherwise would be evenasting. Li et al. [8] recently studied the ground-state lifetime of bound polaron by employing a variational method of the Pekar type in a parabolic quantum dot. A Landau–Pekar variational theory is employed to obtain the ground and the first excited state binding energies of an electron bound to a coulomb impurity in a polar semiconductor quantum dot with parabolic confinement in both two and three dimensions by Chen et al. [9]. K.P. method is used to analyze the electronic structure and intraband optical transitions in self-assembled in GaAs quantum rods in the terahertz range by Prodanovic. Khamkham et al. [10] considering the Landau–Pekar method to study the effect of a magnetic field on the ground-state energy of a donor impurity confined in a polar CdSe spherical quantum dot embedded in a nonpolar matrix. However, the ground-state transition rate of impurity bound polaron in a QR has not been considered so far in these studies.

The purpose of the present paper is to research the ground-state transition probability of impurity bound polaron with strong electron–LO-phonon coupling by utilizing a variational method of Pekar type in a QR. The relations between the ground-state transition probability of impurity bound polaron and the transverse and longitudinal confinement lengths of QR, the ground-state energy, the electron–LO-phonon coupling constant, and the temperature parameter are discussed.

2. Theory

The electron moves in a polar crystal QR with three-dimensional anisotropic harmonic potential. On the basis of the strong-coupled polaron model, the electron–phonon system Hamiltonian with a hydrogen-like impurity at the center can be described:

$$H = H_e + H_{ph} + H_{e-ph} + H_C. \tag{1}$$

$$H_e = \frac{p_{\parallel}^2}{2m^*} + \frac{p_z^2}{2m^*} + V(\rho) + V(z). \tag{2}$$

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where $V(\rho)=(1/2)m\omega_{\parallel}^2\rho^2$ and $V(z)=(1/2)\,m\omega_z^2 z^2$ represent the transverse and longitudinal anisotropic harmonic potentials in the radius and the length directions of the QR, respectively. $\boldsymbol{P}=(\boldsymbol{P}_{\parallel},p_z)$ and m^* denote the momentum and mass of the electron, respectively. The second and third terms in Eq. (1) stand for the local LO-phonon field and the interaction energy of the electron with the LO-phonon. They are given by

$$H_{ph}=\sum_w \hbar\omega_{LO}a_w^+a_w. \tag{3}$$

$$H_{e-ph}=\sum_w[V_w^* a_w^+\exp(-i\boldsymbol{w}\times\boldsymbol{r})+h\times c]. \tag{4}$$

where

$$V_w^*=\frac{i}{\omega}\left(\frac{2\pi e^2\hbar\omega_L}{\varepsilon V}\right)^{1/2}, \tag{5}$$

$$\alpha=\left(\frac{e^2}{2\hbar\omega_{LO}}\right)\left(\frac{2m^*\omega_{LO}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right) \tag{6}$$

here $a_w^+(a_w)$ indicates the creation (destruction) operator of the bulk LO-phonons field with the wave vector $\boldsymbol{w}$ and $\boldsymbol{r}=(\rho,z)$ represents the position vector of an electron, respectively. V plots the volume of the QR. The electron–LO-phonon coupling constant is expressed by α. The last term in Eq. (1) means the coulomb bound potential between the electron and hydrogen-like impurity which can be written as:

$$H_C=-\frac{e^2}{\varepsilon_0|\boldsymbol{r}|} \tag{7}$$

Utilizing Fourier expansion to the coulomb confined potential, it can be represented as:

$$-\frac{e^2}{\varepsilon_0|\boldsymbol{r}|}=-\frac{4\pi e^2}{\varepsilon_0 V}\sum_w\frac{1}{w^2}\exp(-\boldsymbol{w}\times\boldsymbol{r}) \tag{8}$$

We introduce the coordinate transformation, which changes the ellipsoidal boundary into a spherical one [11]: $x'=x,y'=y,z'=z/e'$ where e' shows the ellipsoid aspect ratio and (x',y',z') plots the transformed coordinate. The electron–phonon system Hamiltonian in a new coordinate was changed to H'. And then carry out Lee et al. [12] unitary transformation

$$U=\exp[\sum_w(a_w^+f_w-a_wf_w^*)]. \tag{9}$$

where f_w and f_w^* are variational parameters which will subsequently be chosen by minimizing the energy. We have

$$H^*=U^{-1}H'U \tag{10}$$

The ground-state trial wave function [13] can be denoted

$$|\psi\rangle=\pi^{-(3/4)}\lambda_0^{3/2}\exp\left[-\frac{\lambda_0^2\rho^2}{2}\right]\exp\left[-\frac{\lambda_0^2z^2}{2}\right]|0_{ph}\rangle \tag{11}$$

where $|0_{ph}\rangle$ denotes the zero phonon state and λ_0 is the variational parameter which will subsequently be determined by minimizing the ground-state energy. We then obtain the polaron ground-state energy $E_0=\langle\psi|H^*|\psi\rangle$. Throughout this study, the length and energy of polaron are taken in units of the polaron radius $r_0=(\hbar/2m^*\omega_{LO})^{1/2}$ and the phonon energy constant $R^*=\hbar\omega_{LO}$, the polaron ground-state energy can be written as follow:

$$E_0=(1+\frac{e'^2}{2})\lambda_0^2+\frac{1}{\lambda_0^2l_p^4}+\frac{1}{2\lambda_0^2l_v^4e'^2}-\sqrt{\frac{2}{\pi}}\alpha\lambda_0A(e')-2\sqrt{2}\beta\lambda_0A(e') \tag{12}$$

$l_p=\sqrt{(\hbar/m^*\omega_\parallel)}$ and $l_v=\sqrt{(\hbar/m^*\omega_z)}$ are the transverse and longitudinal confinement lengths, $\beta=(e^2/\varepsilon_0)\sqrt{m^*/\hbar\pi}$ plots the coulomb bound constant. $A(e')$ is expressed as follows:

$$A(e')=\begin{cases}\frac{\arcsin\sqrt{1-e'^2}}{\sqrt{1-e'^2}} & e'<1\\ 1 & e'=1\\ \frac{1}{2\sqrt{e'^2-1}}\ln\frac{e'+\sqrt{e'^2-1}}{e'-\sqrt{e'^2-1}} & e'>1\end{cases} \tag{13}$$

According to the Fermi golden rule, under the affect of the temperature and the electron–phonon interaction, the ground-state transition probability that the polaron transits from the ground-state to the first-excited state after absorbing a LO-phonon is given by

$$P=\frac{\alpha\omega_{LO}}{2\lambda_0}\sqrt{\frac{2m^*\omega_{LO}}{\hbar}}N_w\ln\frac{(\sqrt{\lambda_0^2+2m^*\omega_{LO}/\hbar}+\lambda_0)^2}{(\sqrt{\lambda_0^2-2m^*\omega_{LO}/\hbar}-\lambda_0)^2} \tag{14}$$

In the light of quantum statistics, we get

$$N_w=\left[\exp\left(\frac{\hbar\omega_{LO}}{K_BT}\right)-1\right]^{-1} \tag{15}$$

where the K_B represents Boltzmann constant, and λ means the ground state wave vector of impurity polaron, Eq. (15) should be self-consistent with the N_w of Eq. (14). Moreover, we supposed that $\hbar\omega_{LO}/K_BT=\gamma$ denotes the temperature parameter and then Eq. (15) is turns into $\overline{N}_w=[\exp\gamma-1]^{-1}$.

3. Results and discussion

The dependence of the ground-state transition probability of impurity bound polaron on the transverse and longitudinal confinement lengths of QR, the electron–phonon coupling constant, and the ground-state energy of bound polaron are given in Figs. 1–4.

Fig. 1 illustrates the ground-state transition probability P of impurity bound polaron as a function of the transverse confinement length l_p of QR for different coulomb bound constants $\beta=0.1,0.5,0.7$ and the longitudinal confinement length $l_v=2.5$, the aspect ratio of the ellipsoid $e'=0.5$, the electron–phonon coupling constant $\alpha=6$, and the temperature parameter $\gamma=0.1$. It finds that the ground-state transition probability P of impurity bound polaron increases with enlarging the transverse confinement length l_p of QR. That is because the movement of the electron is confined because the existence of the confine potential in a QR. With enhancing of transverse confinement length, the thermal motion energy of electrons, which take phonon as medium,

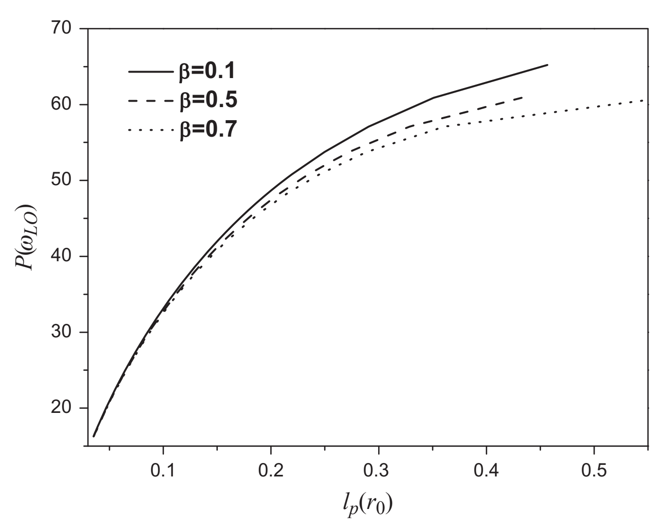

Fig. 1. The ground-state transition probability P of impurity bound polaron as a function of the transverse confinement length l_p for different Coulomb bound constants in a QR.