Temperature and hydrogen-like impurity effects on the excited state of the strong coupling bound polaron in a CsI quantum pseudodot*

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With hydrogen-like impurity (HLI) located in the center of CsI quantum pseudodot (QPD) and by using the variational method of Pekar type (VMPT), we investigate the first-excited state energy (FESE), excitation energy and transition frequency of the strongly-coupled bound polaron in the present paper. Temperature effects on bound polaron properties are calculated by employing the quantum statistical theory (QST). According to the present work's numerical results, the FESE, excitation energy and transition frequency decay (amplify) with raising temperature in the regime of lower (higher) temperature. They are decreasing functions of Coulomb impurity potential strength.

Keywords: temperature effect, bound polaron, CsI quantum pseudodot, quantum statistical theory, excited state

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1. Introduction

The rapid developments in nano-material science and technology have led to the production of low-dimensional quantum structures called quantum dots (QDs).[1] Specifically, QDs are artificial atoms in which electrons are confined in the different potentials. Over the past thirty years, it has been shown theoretically and experimentally that the interaction between electrons and LO-phonons (e-LO-p) is in a strong coupling regime due to electronic energy levels in various material QDs. Many experiments performed on QDs involve energy levels rather than transition between the levels dealing with interaction between e-LO-p from the polarons in the QDs. For instance, by pump-probe mid-infrared spectroscopy, Sauvage *et al.*[2] investigated the dynamics of a polaron in the self-assembled n-doped InAsGaAs QDs. The long T1 decay time of the polaron was measured at both low temperature and room temperature, and its values were around 70 ps and 37 ps. Under optical pumping, and to achieve inter-sublevel population inversion, optical gain, and inter-sublevel polaron laser effect, Sauvage and Boucaud[3] proposed a three-level scheme in self-assembled n-doped InAs/GaAs QDs. Due to electron–phonon (ep) interactions (from polarons), Xu *et al.*[4] studied the mechanisms of quantum dissipation and broadening in self-formed InGaN QDs. The research discovered that a dissipative thermal bath embedded in the QDs is important for photon emission processes. Using the model of multimode Brownian oscillator, it set spontaneous emission spectra model and agreed with experiment and theory in the range of wide temperature. The impurity and the defect usually exist in real crystals. The properties of the crystals can be greatly influenced due to the existence of the impurity and the defect. Zhang *et al.*[5] investigated the effect of topological defects on the transport properties of a narrow ballistic ribbon of graphene with zigzag edges. Zhang and Hu *et al.*[6] found a Kosterlitz–Thouless type metal-to-insulator transition as a function of disorder strength or Fermi energy in disordered graphene with strong long-range impurities. By using a variational method of Pekar type, the Fermi Golden Rule and the quantum statistics theory, we investigate the effects of the hydrogen-like impurity and temperature on the coherence time of a parabolic QD qubit with a hydrogen-like impurity at the center.[7] Furthermore, in theories, by the method of Lee–Low–Pines (LLP) unitary transformation and the VMPT, Khordad[8] derived the expression of bound polaron under Rashba effect in a QPD. Using iterative and compact-density-matrix methods, Khordad[9] also obtained strongly-coupled impurity bound polaron in a QPD. Li *et al.*[10] studied polaron effects on optical absorption coefficients and refractive index changing in the 2D QPD system. From this theoretical research, the polaron properties were studied in various QDs with pseudoharmonic potential (PHP) that includes the harmonic and antidot potentials. Xiao[11] employed the VMPT to study magnetic field effect on RbCl QPD qubit. Sun *et al.*[12] investigated phonons' effects in RbCl QPD qubit. Previous study of the most important polarons in QPD focused on the calculation of polarons state energies at zero temperature. Actually, the experiments for the state energies in physical system are performed at finite temperature, and consider that finite temperature is significant. Therefore it is very important to investigate the polaron state energies' temperature effect. Using the QST, Chen *et al.*[13,14] investigated the effect of temperature on the probability density of the electron in parabolic QD qubit and the parabolic

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linear bound potential and Coulomb bound potential QD qubit. Li *et al.*[15] employed the same method to study the effect of temperature on magnetopolaronic vibrational frequency in an anisotropic QD. Sun *et al.*[16] studied the temperature effect on the FESE and transition frequency of a strongly-coupled polaron in symmetrical RbCl QD by using linear combination operator and the QST. For more information about temperature and polarons see the reference listed in Refs. [17]–[19]. However, the temperature effects on the strongly-coupled bound polaron properties in a CsI QPD have not been studied by employing the VMPT and QST so far.

In the present article, we thoroughly investigate the temperature effects and Coulomb impurity potential strength on the strongly-coupled bound polaron properties in CsI QPD with VMPT and QST. The research results have important theoretical significance, and are useful and meaningful for the implementation of low-dimensional quantum devices.

2. Theory model's description

Considering a QPD of CsI crystal in the presence of electron-bulk longitudinal optical (LO) phonon interaction, an electron is bound to a HLI in the system, and is subjected to a pseudoharmonic potential (PHP). Within the framework of effective mass approximation, the Hamiltonian of the electron–phonon system takes the following form of

$$\begin{aligned} H &= \frac{p^2}{2m} + V(r) + \sum_{\boldsymbol{q}} \hbar\omega_{\rm LO} a_{\boldsymbol{q}}^{\dagger} a_{\boldsymbol{q}} \\ &\quad + \sum_{\boldsymbol{q}} [V_q a_{\boldsymbol{q}} \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}) + \text{h.c.}], \end{aligned} \tag{1}$$

where

$$V(r) = V_0 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2, \tag{2}$$

where the physical quantities' significances in Eq. (1) are according to Ref. [20]. $-\beta/r$ denotes the Coulomb potential between the HLI and the electron. $\beta = e^2/\varepsilon_0$ is the Coulomb impurity potential strength. $V(r)$ is the PHP[21] that includes both harmonic and antidot potentials. V_0 and r_0 are the chemical potential of the two-dimensional electron gas (TDEG) and the PHP zero point, respectively.

According to the VMPT[22,23] and the Ref. [24], the trial wavefunction is given by

$$|\psi\rangle = |\varphi\rangle U |0_{\rm ph}\rangle, \tag{3}$$

with $|\varphi\rangle$ depending only on the coordinate of electron, $|0_{\rm ph}\rangle$ being the vacuum state of phonon with $a_{\boldsymbol{q}}|0_{\rm ph}\rangle = 0$, and $U|0_{\rm ph}\rangle$ denoting the coherent state of the phonon,

$$U = \exp\left[\sum_{\boldsymbol{q}} \left(a_q^{\dagger} f_q - a_{\boldsymbol{q}} f_q^* \right) \right], \tag{4}$$

where $f_{\boldsymbol{q}}$ ($f_{\boldsymbol{q}}^*$) is the variational function, we choose the trial polaron's wavefunction of the ground and the first excited states (GFES) as[25]

$$|\varphi_0(\lambda_0)\rangle = |0\rangle |0_{\rm ph}\rangle = \pi^{-3/4} \lambda_0^{3/2} \exp\left[-\frac{\lambda_0^2 r^2}{2} \right] |0_{\rm ph}\rangle, \tag{5}$$

$$\begin{aligned} |\varphi_1(\lambda_1)\rangle &= |1\rangle |0_{\rm ph}\rangle = \left(\frac{\pi^3}{4} \right)^{-1/4} \lambda_1^{5/2} r\cos\theta \exp\left(-\frac{\lambda_1^2 r^2}{2} \right) \\ &\quad \times \exp(\pm \mathrm{i}\phi) |0_{\rm ph}\rangle, \end{aligned} \tag{6}$$

where λ_0 and λ_1 are the variational parameters. The polaron FESE and the excitation energy in the CsI QPD can be described as

$$\begin{aligned} E_1(\lambda_1) &= \frac{5\hbar^2}{4m}\lambda_1^2 + \frac{5V_0}{2\lambda_1^2 r_1^2} + \frac{2}{3}V_0\lambda_1^2 r_0^2 - 2V_0 \\ &\quad - \frac{3\sqrt{2}}{4\sqrt{\pi}}\alpha\hbar\omega_{\rm LO}\lambda_1 R_0 - \frac{4\beta}{3\sqrt{\pi}}\lambda_1, \end{aligned} \tag{7}$$

$$\begin{aligned} \Delta E &= E_1 - E_0 \\ &= \frac{5\hbar^2}{4m}\lambda_1^2 - \frac{3\hbar^2}{4m}\lambda_0^2 + \frac{5V_0}{2\lambda_1^2 r_1^2} - \frac{3V_0}{2\lambda_0^2 r_0^2} + \frac{2}{3}V_0\lambda_1^2 r_0^2 \\ &\quad - 2V_0\lambda_0^2 r_0^2 - \frac{3\sqrt{2}}{4\sqrt{\pi}}\alpha\hbar\omega_{\rm LO}\lambda_1 R_0 \\ &\quad + \frac{\sqrt{2}}{\sqrt{\pi}}\alpha\hbar\omega_{\rm LO}\lambda_0 R_0 - \frac{4\beta}{3\sqrt{\pi}}\lambda_1 + \frac{2\beta}{\sqrt{\pi}}\lambda_0, \end{aligned} \tag{8}$$

where $R_0 = (\hbar/2m\omega_{\rm LO})^{1/2}$ plots the polaron radius. The transition frequency of the strong-coupling polaron in the CsI QPD is obtained as

$$\omega = \frac{\Delta E}{\hbar}. \tag{9}$$

The LO phonons' mean number around the electron can be described as

$$\begin{aligned} N &= \langle\psi_0| U^{-1} \sum_{\boldsymbol{q}} a_{\boldsymbol{q}}^{\dagger} a_{\boldsymbol{q}} U |\psi_0\rangle \\ &= \frac{1}{\sqrt{2\pi}}\alpha R_0\lambda_0 + \frac{3}{4\sqrt{2\pi}}\alpha R_0\lambda_1. \end{aligned} \tag{10}$$

3. Temperature effects

At finite temperature and with HLI in the center of the CsI QPD, the different states' statistical average value can be described by the strongly-coupled bound polaron properties. According to the QST, the bulk LO phonons' statistical average number can be expressed as

$$\bar{N} = [\exp(\hbar\omega_{\rm LO}/K_{\rm B}T) - 1]^{-1} \tag{11}$$

with $K_{\rm B}$ and T being the Boltzmann constant and the system temperature, respectively. Through self-consistent calculation about Eq. (10) and Eq. (11), we investigate the relation between the two variational parameters λ_0, λ_1 and temperature T. In Eqs. (7), (8), and (9), we found that the FESE, excitation energy and transition frequency of polaron depends on not only the variational parameters λ_0 and λ_1, but also relates to the temperature T.

4. Results and discussions

In the following content, numerical results for the parameters of a CsI QPD crystal system and the parameters used in our calculations are $\hbar\omega_{\rm LO} = 11.22845266$ meV, $m = 0.42m_0$, and $\alpha = 3.67$.[26]

With HLI in the center of a CsI QPD, the FESE of strongly-coupled polaron as the function of the temperature has been depicted in Fig. 1 for four different strengths of the Coulomb impurity potential, i.e., $\beta = 5.0$, 10.0, 15.0, and 20.0 meV·10^{-8} m, respectively. The TDEG chemical potential V_0 is set to be 10.0 meV, the PHP zero point $r_0 = 12.0$ nm and the polaron radius $R_0 = 4.0$ nm.

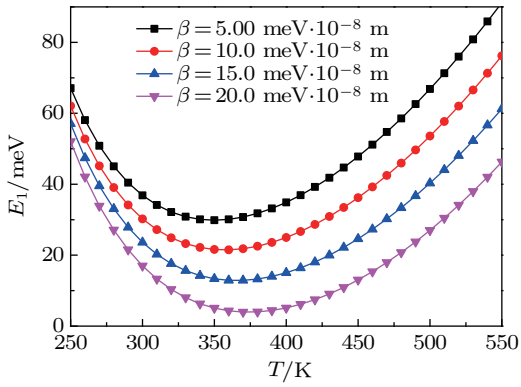


Fig. 1. (color online) First-excited state energy E_1 versus temperature T and Coulomb impurity potential strength β.

To observe the temperature effects and the Coulomb impurity potential strength on the polaron excitation energy in the CsI QPD, we set $V_0 = 10.0$ meV, $R_0 = 4.0$ nm, and $r_0 = 12.0$ nm in Fig. 2, we note that the excitation energy of polaron varying with the temperature and the Coulomb impurity potential strength. Figure 3 displays the transition frequency dependence on the temperature and the Coulomb impurity potential strength for $V_0 = 10.0$ meV, $R_0 = 4.0$ nm, and $r_0 = 12.0$ nm.

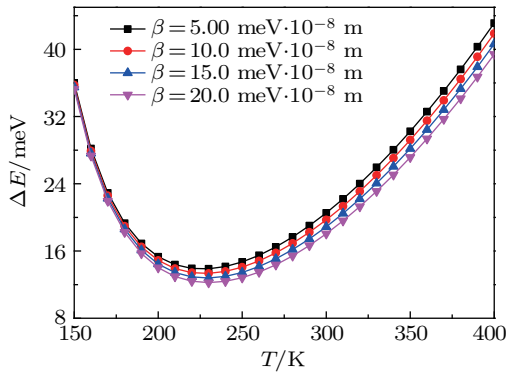


Fig. 2. (color online) Excitation energy ΔE versus temperature T and Coulomb impurity potential strength β.

As is seen from Figs. 1, 2, and 3, the FESE, excitation energy and transition frequency decrease as the temperature is enhanced in the lower region of temperatures, and it increases as the temperature is enhanced in the higher region of temperatures. The reasons are as follow: the electrons' and phonons' velocities are increased with the enhancement of the temperature, and then the electrons interact with more phonons. The contribution from electrons with increased velocity, which makes more and more electrons locate on the ground- and first-excited-states, is not as big as that from the electrons interacting with more phonons to destruct these states in the region of lower temperature. Thus the FESE, excitation energy and transition frequency are decayed. However, the contributions from the electron velocity and the ep interaction are reversed and lead to the increase of the three physics quantities at finally in higher temperature region.

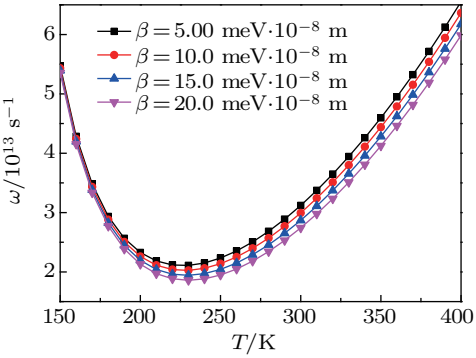


Fig. 3. (color online) Transition frequency ω versus temperature T and Coulomb impurity potential strength β.

As noted in Figs. 1, 2, and 3, the FESE, excitation energy and transition frequency decrease with increasing Coulomb impurity potential strength. Coulomb impurity potential equals a new confinement on the electron, resulting in the greater overlapping between the electron wavefunction with each other, the ep interactions and the electron energy will be amplified, and the FESE, excitation energy and transition frequency are enhancing functions of Coulomb impurity potential strength. However the last term in Eq. (7) and the last two terms in Eq. (8) are the contribution of Coulomb impurity potential to the FESE and excitation energy, which is a negative value, whereas the total FESE and excitation energy are positive values. Therefore, they are its decaying functions.

Here we suggest two ways to control the FESE, excitation energy and transition frequency in the CsI QPD via adjusting the temperature and adjusting the Coulomb impurity potential strength.

Moreover, the technique of controlling the temperature and Coulomb impurity potential strength may be used for building quantum information devices, which is in agreement with the results of Ji *et al.*[27]

5. Conclusions

The impurity and temperature effects on the FESE, excitation energy and transition frequency of bound polaron strongly-coupled with the HLI in the center of CsI QPD have

been investigated. Calculations were performed by using QST and VMPT. The results were illustrated as functions of the temperature and the Coulomb impurity potential strength. It has been seen that the FESE, excitation energy and transition frequency decrease (increase) with increasing temperature in the regime of lower (higher) temperature, and they decreased with enhanced Coulomb impurity potential strength. The temperature, the pseudoharmonic and Coulomb impurity potentials are important factors for studying the polaron states' properties in the CsI QPD with HLI located in the center of the system.

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