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Temperature effect on vibrational frequency and ground state energy of strong-coupling polaron in symmetry RbCl quantum dots

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Abstract. By employing the linear combination operator and the unitary transformation methods, we study the vibrational frequency and the ground state energy of a strong-coupling polaron in symmetric RbCl quantum dots (SRQDs). The effects of the temperature and the confinement strength are taken into account. It is found that the vibrational frequency and the ground state energy are increasing functions of the temperature and the confinement strength. We find two ways of tuning the vibrational frequency and the ground state energy via adjusting the temperature and the confinement strength.

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Key words: vibrational frequency, linear combination operator, temperature effect, unitary transformation methods, Polaron.

1 Introduction

In recent years, there has been an active research subject in the experimental and theoretical physicists study of low-dimensional nanostructures. This low-dimensional nanostructures are not only advantageous to the point view of fundamental physics but also electronic and optoelectronic devices [1,2]. Consequently, there has been a large amount of experimental work [3-5] on QD. Meanwhile, many investigators studied its properties in many aspects by a variety of theoretical methods [6-8]. Using the framework of effective mass theory, Wang and Li [9] theoretically investigated the center-of-mass motion of quasi-two-dimensional excitons with spin-orbit coupling. Using a variational method of the Pekar type, Xiao [10] study the ground and first excited states energies and the corresponding transition frequency of a strong-coupling polaron in an asymmetric quantum

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dot (AQD). Beard [11] uses a way to enhance solar energy conversion by utilizing the excess energy in the absorbed photons to study Multiple exciton generation in quantum dots. Based on the variational method of Pekar type, state energies and transition frequency of strong-coupling polaron in an anisotropic quantum dot had been calculated by us [12].

In this paper, by using the linear combination operator and unitary transformation methods, we study the temperature effect on vibrational frequency and ground state energy of a strong-coupling polaron in a SRQD.

2 Theory model calculations

The electron under consideration is moving in a crystal RbCl quantum dot with the parabolic potential which is much more confined in z direction than in the x–y directions, and interacting with bulk LO phonons. The Hamiltonian of the electron-phonon interaction system can be written as

$$H=\frac{p^2}{2m}+\sum_{\mathbf{q}}\hbar\omega_{LO}\alpha_q^+\alpha_q+\frac{1}{2}m\omega_{\|}^2\rho^2+\frac{1}{2}m\omega_z^2z^2+\sum_q[V_q\alpha_q\exp(i\mathbf{q}\cdot\mathbf{r})+h.c.] \tag{1}$$

where m is the band mass, ω_o is the magnitude of the confinement strengths of the potentials in the x-y plane, respectively. $a_{\mathbf{q}}^+(a_{\mathbf{q}})$ denotes the creation (annihilation) operator of the bulk LO phonon with wave vector $\mathbf{q}$, P and $\mathbf{r}$=($\mathbf{p}$,z) is the momentum and position vector of the electron. V_q and α in Eq. (1) are

$$V_q=i\left(\frac{\hbar\omega_{LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{LO}}\right)^{\frac{1}{4}}\left(\frac{4\pi\alpha}{V}\right)^{\frac{1}{2}},\quad \alpha=\left(\frac{e^2}{2\hbar\omega_{LO}}\right)\left(\frac{2m\omega_{LO}}{\hbar}\right)^{\frac{1}{2}}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_o}\right) \tag{2}$$

Then, we carry out the unitary transformation to Eq. (1):

$$U=\exp\left[\sum_{\mathbf{q}}\left(f_q\alpha_{\mathbf{q}}^+-f_q^*\alpha_{\mathbf{q}}\right)\right], \tag{3}$$

where f_q and f_q are the variation functions, we introduce a linear combination operator:

$$\begin{aligned} p_j&=\left[\tfrac{m\hbar\lambda}{2}\right]^{\frac{1}{2}}\left(b_j+b_j^+\right)\\ r_j&=i\left[\tfrac{\hbar}{2m\lambda}\right]^{\frac{1}{2}}\left(b_j-b_j^+\right)\end{aligned},\quad j=x,y \tag{4}$$

where λ is the variation parameter which describing the vibrational frequency of polaron. The ground state wave function of the system is chosen as

$$|\psi_0\rangle=|\varphi(z)\rangle|0\rangle_a|0\rangle_b, \tag{5}$$

$|0\rangle_a$ refers to the unperturbed zero phonon state and $|0\rangle_b$ denotes the vacuum state of the b operator. By calculating, we have

$$\lambda^2-\frac{\alpha}{3}\sqrt{\frac{\omega_{LO}}{\pi}}\lambda^{\frac{3}{2}}-\omega_0^2=0, \tag{6}$$

The ground state energy, first-excited state energy can be written as

$$E_0=\frac{\hbar}{2}\lambda+\frac{\hbar\omega_0^2}{2\lambda}-\frac{1}{3}\alpha\hbar\sqrt{\frac{\omega_{LO}\lambda}{\pi}}. \tag{7}$$

Where ω_0 is the quantum dot confinement strength. The mean number of phonons of the ground state around the electron is

$$N=\langle\psi|U^{-1}\alpha_q^+\alpha_q U|\psi\rangle=\frac{\alpha}{3\sqrt{\pi}}\sqrt{\frac{\lambda}{\omega_{LO}}}. \tag{8}$$

3 Temperature effects

At finite temperature, electron-phonon system is no longer entirely in the ground state. The lattice vibrations excite not only the real phonon but also electron in a parabolic potential. According to the quantum statistics theory, the mean number of phonons is

$$\bar{N}=\left[\exp\left(\frac{\hbar\omega_{LO}}{k_BT}\right)-1\right]^{-1}. \tag{9}$$

where k_B is the Boltzmann constant. With the consideration mentioned above, the values of λ determined by Eq. (8) relates not only to the value of N but also to the value $\vec{N}$, which should be self-consistent calculated with Eq. (9). In such a way, we can see that the vibrational frequency, the ground state energy and the optical phonons mean number of the polaron all depend on the variational parameter λ, and then are related to the temperature T.

4 Results and discussion

Below we preset numerical calculations to show the effects of the temperature and confinement strength on the vibrational frequency and the ground state energy of the polaron in a SRQD. Choosing the RbCl crystals, as examples, we perform the numberical evaluation. The experiment paramenters used in the calculation are α=3.81, $\hbar\omega_{LO}$=21.45 meV. The numerical results are given in Figs. 1-2.

Fig. 1 indicates the vibrational frequency λ as functions of the confinement strength ω_0 and the temperature T. From Fig. 1 can see that the vibrational frequency is an increasing function of the temperature and the confinement strength.

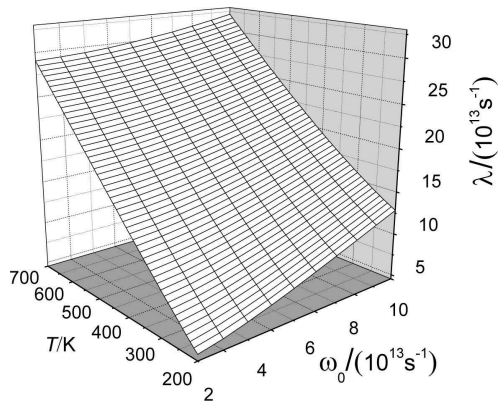

Figure 1: The relations of the variation parameter with the confinement strength and the temperature .

Fig. 2 depicts the ground state energy E_0 as functions of the confinement strength ω_0 and the temperature T. From Fig. 2 can see that the ground state energy increases with increasing the temperature and the confinement strength. Meanwhile, from Fig. 1 and Fig. 2 we can see that the vibrational frequency and the ground state energy are increasing functions of the temperature. This is because that higher temperature increases the speed of heat sport of the electron and the phonon, so that the electron will interact with more phonons. For this reason, the vibrational frequency and the ground state energy will be enhanced with increasing temperature. We suggest a new way of tuning the SRQD vibrational frequency and ground state energy via adjusting the temperature. From Fig. 1 and Fig. 2 we also find that the vibrational frequency and the ground state energy are increasing functions of the confinement strength. Since the motion of the electrons is confined by the confining potential, with the increase of the confinement strength

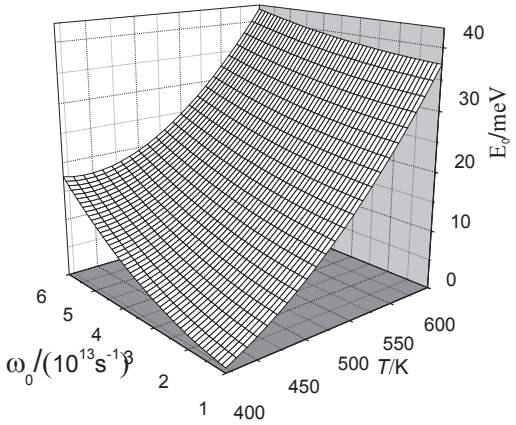

Figure 2: The relations of the ground state energy E_0 with the confinement strength ω_0 and the temperature T.

(ω_0) increase, the thermal motion energy of the electrons and the interaction between an electron and the phonons , which take phonons as the medium, are enhanced because of a smaller range of particle motion. As a result of it, the vibrational frequency and the ground state energy with the increase of the confinement strength. Those attribute to interesting quantum size confining effects. We also find the second way of tuning the SRQD vibrational frequency and the ground state energy via adjusting the confinement strength.

5 Conclusion

In conclusion, based on the linear combination operator and the unitary transformation methods, we have investigated the vibrational frequency and the ground state energy of the strong-coupling polaron in SRQDs. It is found that the vibrational frequency and the ground state energy are increasing functions of the temperature and the confinement strength. We find two ways of tuning the vibrational frequency and the ground state energy via adjusting the temperature and the confinement strength.

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References

[1] Y. Li, F. Qian, and J. Xiang, Mater. Today 9 (2006)18.
[2] S. Roquet, A. Cravino, P. Leriche, O. Aleveque, P. Frere, and J. Roncali, J. Am. Chem. Soc. 128 (2006) 3459.
[3] I. S. Grudinin, H. Lee, O. Painter, and J. V. Kerry, Phys. Rev. Lett. 104 (2010) 083901.
[4] C. M. Wu, T. W. Liu, M. H. Wu, R. K. Lee, and W. Y. Cheng, Org. Lett. 38 (2013) 3186.
[5] N. Akopian, L. Wang, A. Rastelli, O. G. Schmidt, and V. Zwiller, Nature Photon. 5 (2011)230.
[6] C. Matthiesen, A. N. Vamivakas, and M. Atat*ü*re. Phys. Rev. Lett. 108 (2012) 093602.
[7] W. B. Gao, P. Fallahi, E. Togan, J. Miguel-Sanchez, and A. Imamoglu, Nature 491(2012)426.
[8] I. Buluta, S. Ashhab, and F. Nori, Rep. Prog. Phys. 74 (2011) 104401.
[9] J. W. Wang and S. S. Li, Appl. Phys. Lett. 92 (2008) 012106.
[10] J. L. Xiao, J. Low Temp. Phys. 172 (2013) 122.
[11] A. J. Nozik, Chem. Phys. Lett. 457 (2008) 3.
[12] Y. Sun, Z. H. Ding, and J. L. Xiao, J. At. Mol. Sci. 4 (2013) 176.