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State energies and transition frequency of strong-coupling polaron in an anisotropic quantum dot

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Abstract. We study the ground and the first excited states energies and the transition frequency between the first excited- and the ground-state of strong-coupling polaron in an anisotropic quantum dot. The effects of the electron-phonon coupling strength and the transverse and the longitudinal effective confinement lengths are taken into consideration by using variational method of the Pekar type. It is found that the transition frequency is an increasing function of the electron-phonon coupling strength, whereas the state energies are decreasing one of it. They will increase rapidly with decreasing transverse and longitudinal effective confinement lengths.

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Key words: Anisotropic quantum dot, polaron, Variational method of the Pekar type

1 Introduction

In recent years, lots of novel effects in systems consisting of quantum dot (QD) have attracted interests from more and more physicists. Because of the wide device applications and many new effects in such structures, understanding their electronic and transport properties is of particular importance. Consequently, there has been a large amount of experimental work [1-3] on QD. Meanwhile, many investigators studied its properties in many aspects by a variety of theoretical methods [4-8]. Using a variational approach with squeezed states, Kervan *et al.* [9] investigated the polaronic effects of an electron confined in a parabolic QD and obtained the polaronic correction to the ground and the first excited states energies in the presence of optical phonons. Li and Xia [10]studied the quantum-confined Stark effects in GaAs/$Al_xGa_{1-x}As$ self-assembled QDs in the framework of the effective-mass envelope-function theory. The electron and hole optical transition energies were calculated in the presence of an electric field in different directions. At

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low temperature, Zaitsev *et al.* [11] studied the magneto-optics and picosecond dynamics of radiative recombination of excitons in self-assembled semi-magnetic CdSe /ZnMnSe QDs. Kaer *et al.* [12] investigated the influence of the electron-phonon interaction on the dynamical properties of a QD-cavity system. Within the spin-density-functional theory, Zhang *et al.*[13] investigated the electronic structure of dynamic QDs formed by surface acoustic waves potential and the confinement potential produced by gate voltage. Based on Huybrechts's strong-coupled polaron model, Tokuda modified the linear-combination operator and the unitary transformation methods. The effective mass of strong-coupled polaron in an asymmetric QD induced by Rashba effect has been studied by us [14]. The properties of the strong-coupling polaron in an anisotropic quantum dot, however, has not been studied so far by employing variational method of the Pekar type. Especially, the properties of the transition frequency of the polaron have never been investigated yet.

In the present paper, we study the effects of the electron-phonon coupling strength and the transverse and longitudinal effective confinement lengths on the ground and the first excited states energies and the transition frequency of a strong-coupling polaron in an anisotropic quantum dot by using variational method of the Pekar type.

2 Theory model and calculations

The electron under consideration is moving in a polar crystal quantum dot with three-dimensional anisotropic harmonic potential, and is interacting with bulk LO phonons. The Hamiltonian of the electron-phonon interaction system can be written as

$$H=\frac{p^2}{2m}+\sum_{\mathbf{q}}\hbar\omega_{LO}a_{\mathbf{q}}^{+}a_{\mathbf{q}}+\frac{1}{2}m\omega_{||}^2\rho^2+\frac{1}{2}m\omega_z^2z^2+\sum_{\mathbf{q}}[V_{\mathbf{q}}a_{\mathbf{q}}\exp(i\mathbf{q}\cdot\mathbf{r})+hc], \tag{1}$$

where m is the band mass, $\omega_{||}$ and ω_z are the measure of the transverse and longitudinal confinement strengths of the potentials in the xy plane and the z direction, respectively. $a_{\mathbf{q}}^{+}(a_{\mathbf{q}})$ denotes the creation (annihilation) operator of the bulk LO phonon with wave vector $\mathbf{q}$, and $\mathbf{r}=(\rho,z)$ is the position vector of the electron. V_q and α in Eq.(1) are

$$\begin{aligned} V_q&=i\left(\frac{\hbar\omega_{LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{LO}}\right)^{\frac{1}{4}}\left(\frac{4\pi\alpha}{v}\right)^{\frac{1}{2}},\\ \alpha&=\left(\frac{e^2}{2\hbar\omega_{LO}}\right)\left(\frac{2m\omega_{LO}}{\hbar}\right)^{\frac{1}{2}}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right). \end{aligned} \tag{2}$$

We carry out the well known Lee-Low-Pines [15] transformation to Eq. (1)

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

where $f_q(f_q^*)$ is the variational function, we obtain

$$H' = U^{-1}HU. \tag{4}$$

For convenience, we use spherical coordinates and then the ground state wave function is a Gaussian. Following the Pekar variational method, we may choose the trial ground state wavefunction of the electron-phonon system to be

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

where λ_0 is the variational parameter, $|0_{ph}\rangle$ is unperturbed zero phonon state, which satisfies $a_{\mathbf{q}}|0_{ph}\rangle = 0\cdot|0\rangle$ is the trial ground state wavefunction of electron. Similarly, the trial wave-function of the electron-phonon system in the first-excited state may be chosen as

$$|\varphi_1\rangle = |1\rangle|0_{ph}\rangle = \left(\frac{\pi^3}{4}\right)^{-\frac{1}{4}}\lambda_1^{\frac{5}{2}} r\cos\theta\exp\left(-\frac{\lambda_1^2 r^2}{2}\right)|0_{ph}\rangle, \tag{6}$$

where λ_1 is the variational parameter and $|1\rangle$ is the first excited state trial wavefunction of electron with $\langle 0|0\rangle = 1$, $\langle 1|1\rangle = 1$, $\langle 1|0\rangle = 0$. The above equation satisfies the following normalized relation:

$$\langle\varphi_0|\varphi_0\rangle = 1,\ \langle\varphi_0|\varphi_1\rangle = 0,\ \langle\varphi_1|\varphi_1\rangle = 1. \tag{7}$$

By minimizing the expectation value of the Hamiltonian, we then obtain the electron ground state energy $E_0 = \langle\varphi_0|H'|\varphi_0\rangle$ and the first excited state energy $E_1 = \langle\varphi_1|H'|\varphi_1\rangle$. By using the variational method, we can obtain λ_0 and λ_1, and the ground state and first-excited state energies of the polaron in the anisotropic QD can be written as

$$E_0(\lambda_0) = \frac{3}{2}\lambda_0^2 + \frac{1}{\lambda_0^2 l_p^4} + \frac{1}{2\lambda_0^2 l_v^4} - \sqrt{\frac{2}{\pi}}\alpha\lambda_0, \tag{8}$$

$$E_1(\lambda_1) = \frac{5}{2}\lambda_1^2 + \frac{1}{\lambda_1^2 l_p^4} + \frac{3}{2\lambda_1^2 l_v^4} - \frac{3\alpha}{2\sqrt{2\pi}}\lambda_1, \tag{9}$$

where $l_p = \sqrt{\hbar/m\omega_{||}}$ and $l_v = \sqrt{\hbar/m\omega_z}$ are the transverse and longitudinal effective confinement lengths. The transition frequency between the first excited and the ground states of the polaron is given by

$$\omega = \frac{E_1 - E_0}{\hbar}. \tag{10}$$

3 Numerical results and discussion

Now we perform numerical calculations to show the effects of the electron-phonon coupling strength α and the transverse and longitudinal effective confinement lengths l_p and

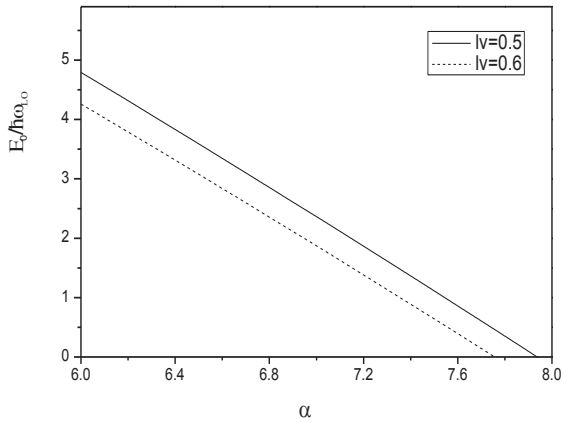

Figure 1: The ground state energy E_0 as a function of the electron-phonon coupling strength α.

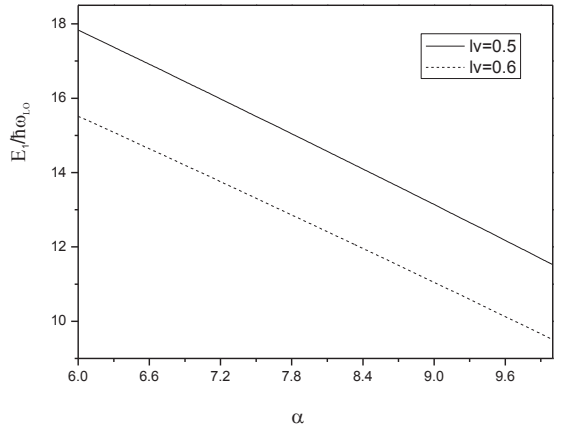

Figure 2: The first excited state energy E_1 as a function of the electron-phonon coupling strength α.

l_v on the polaron ground state energy E_0, the first excited state energy E_1 and the transition frequency ω.

Figs. 1, 2 and 3 show the relationship between E_0, E_1 and ω of the polaron varying with the electron-phonon coupling strength α for $l_p = 0.4$. The solid and the dotted lines correspond to the cases of $l_v = 0.5$ and $l_v = 0.6$, respectively. From the three figures we can see that E_0, E_1 are decreasing functions of the electron-phonon coupling strength α, whereas the transition frequency ω is an increasing one of the coupling strength α. This is because the larger the electron-phonon coupling strength is, the stronger the electron-phonon interaction is. Therefore, it leads to the electron energy increment and makes the electrons interact with more phonons. As a result of it, the transition frequency of the polaron is increased. Since the fourth term in Eqs. (8) and (9) are the contribution from the electron-phonon coupled to the state energies with a negative value. For this reason, the state energies will be enhanced with decreasing coupling strength.

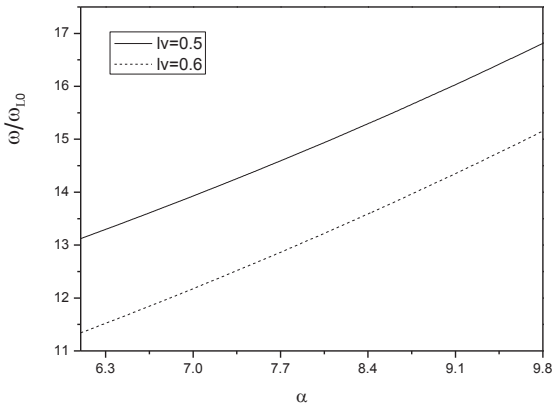

Figure 3: The transition frequency ω as a function of the electron-phonon coupling strength α.

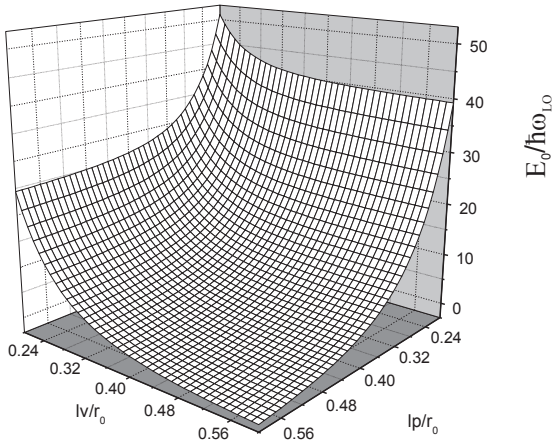

Figure 4: The ground state energy E_0 as a function of the transverse and longitudinal effective confinement lengths l_p and l_v.

Figs. 4, 5 and 6 present E_0, E_1 and ω as functions of the transverse and longitudinal effective confinement length l_p and l_v with $\alpha = 6.5$. From the three figures we can see that the ground and first excited states energies and the transition frequency increase rapidly with decreasing transverse and longitudinal effective confinement lengths. This result is in agreement with that of the vibrational frequency and the interaction energy of Ref.16. From the expressions of $l_p = \sqrt{\hbar/m\omega_{||}}$ and $l_v = \sqrt{\hbar/m\omega_z}$, we can see that the effective confinement lengths (l_p and l_v) are reciprocal with the square root of the confinement strength $\omega_{||}$ and ω_z, and then the state energies and the transition frequency will increase with increasing confinement strength. This is because the motion of the electrons is confined by the confining potential. With the increase of the confining potential ($\omega_{||}$ and ω_z), that is, with decreasing ρ and z, the energy of the electrons and the interaction between

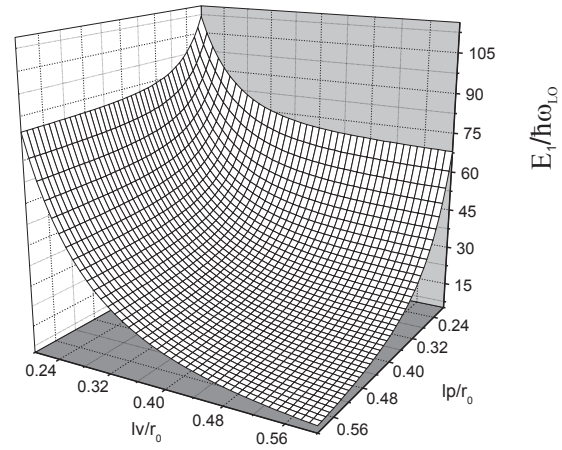

Figure 5: The first excited state energy E_1 as a function of the transverse and longitudinal effective confinement lengths l_p and l_v.

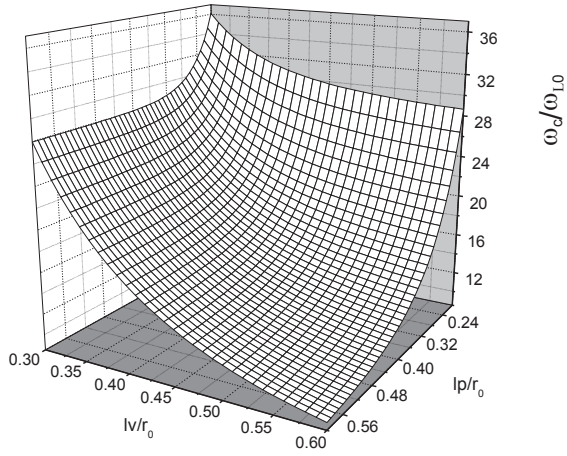

Figure 6: The transition frequency ω as a function of the transverse and longitudinal effective confinement lengths l_p and l_v.

the electron and the phonons are enhanced because of the smaller particle motion range. As a result of it, the state energies and the transition frequency of the polaron are all increased. These can also be attributed to the interesting quantum size confining effects. We also see that the influence of the transverse confinement length on them is larger than that of the longitudinal one.

4 Conclusion

In conclusion, based on the Pekar type variational method, we have investigated the ground and the first excited states energies and the transition frequency of the strong-

coupling polaron in an anisotropic quantum dot. It is found that the state energies are decreasing functions of the electron-phonon coupling strength, whereas the transition frequency is an increasing one of it. They will increase rapidly with decreasing transverse and longitudinal effective confinement lengths. These can also be attributed to the interesting quantum size confining effects.

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References

[1] A.I. Yakimov, A.V. Dvurechenskii, G.M. Min,kov, A.A. Sherstobitov, A.I. Nikiforov, and A.A. Bloshkin, J. Exp. Theor. Phys. 100 (2005) 722.
[2] J. R. Santos, M. I. Vasilevskiy, and S. A. Filonovich, Phys. Rev. B 78 (2008) 245422.
[3] V. G. Storchak, O. E. Parfenov, J. H. Brewer, P. L. Russo, S. L. Stubbs, R. L. Lichti, D. G. Eshchenko, E. Morenzoni, T. G. Aminov, V. P. Zlomanov, A. A. Vinokurov, R. L. Kallaher, and S. V. Molnar, Phys. Rev B 80 (2009) 235203.
[4] F. Arciprete, M. Fanfoni, F. Patella, A.D. Pia, A. Balzarotti, and E. Placidi, Phys. Rev. B 81 (2010) 165306.
[5] K. Sellami and S. Jaziri, Physica E 26 (2005) 143.
[6] S. S. Li and J. B. Xia, J. Appl. Phys. 101 (2007) 091736.
[7] F. Baruffa, P. Stano, and J. Fabian. Phys. Rev. Lett. 104 (2010) 126401.
[8] Z. X. Li, Z. H. Ding, and J. L. Xiao, J. Low. Temp. Phys. 159 (2010) 592.
[9] N. Kervan, T. Altanhan, and A. Chatterjee, Phys. Lett. A 315 (2003) 280.
[10] S. S. Li and J. B. Xia, Appl. Phys. Lett. 87 (2005) 043102.
[11] S. V. Zaitsev, H. Schomig, A. Forchel, and G. Bacher, JETP. Lett. 85 (2007) 323.
[12] P. Kaer, T. R. Nielsen, P. Lodahl, A. P. Jauho, and J. Mork, Phys. Rev. Lett. 104 (2010) 157401.
[13] W. Zhang, J. Gao, H.-J. Guo, and C.-Y. Zhang, Eur. Phys. J. B 79 (2011) 351.
[14] Z. X. Li, J. L. Xiao, and H. Y. Wang, Mod. Phys. Lett. B 24 (2010) 2423.
[15] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. 90 (1953) 297.
[16] W. Xiao and J. L. Xiao, Mod. Phys. Lett. B 23 (2009) 2449.