Ground-state energy of weak-coupling polarons in quantum rods*

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Abstract: The Hamiltonian of the quantum rod (QR) with an ellipsoidal boundary is given after a coordinate transformation. Using the linear-combination operator and unitary transformation methods, the vibrational frequency and the ground-state energy of weak-coupling polarons are obtained. Numerical results illustrate that the vibrational frequency increases with the decrease of the effective radius R_0 of the ellipsoidal parabolic potential and the aspect ratio e' of the ellipsoid, and that the ground-state energy increases with the decrease of the effective radius R_0 and the electron-LO-phonon coupling strength α. In addition, the ground-state energy decreases with increasing aspect ratio e' within $0 < e' < 1$ and reaches a minimum when $e' = 1$, and then increases with increasing e' for $e' > 1$.

Key words: quantum rod; weak-coupling; linear-combination operator; polaron
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1. Introduction

In recent years, with the rapid development of molecular beam epitaxy and metal organic chemical vapor deposition, various quantum dots (QDs)[1, 2] have already been produced. They have potential applications in novel quantum functional devices because of their unique photoelectric and transport properties. Therefore, the problem of polarons in low-dimensional systems has been attracting people's attention[3]. Oshiro *et al.*[4] studied the polaron in a spherical QD embedded in a nonpolar matrix using a variational method. They concluded that with the increase in the dot radius the magnitude of the polaron energy shift decreases rapidly from a large value and then gradually approaches the bulk value. Zhao *et al.*[5] studied the properties of a weak-coupling magnetopolaron in a cylindrical QD using a linear-combination operator and unitary transformation methods. Pokatilov *et al.*[6] analyzed the basic polaron parameters–the ground-state energy, the polaron effective mass, the number of phonons in the polaron cloud, and the polaron radius–for a three-axis ellipsoidal in a potential well. In addition, many researchers have researched the properties of quantum rods (QRs) in the past several years. Comas *et al.*[7] studied the surface polar-optical phonons for semiconductor QRs and discussed the differences between spherical and quasi-spherical QDs. Zhang *et al.*[8] investigated the effects of the shape and the magnetic field on the linear polarization factors in the framework of the effective-mass envelop function theory. Li and Wang[9]calculated the high energy excitations of QRs using the plane-wave pseudopotential method. Li and Xia[10, 11] studied the electronic structure and optical properties of QRs and the effects of the electric field on the electronic structure and the optical properties of QRs. However, so far, only a small amount of work has been done on the ground state energy of polarons by the linear-combination operator method.

In this paper, the influence of the parabolic confined potential with an ellipsoidal boundary condition on the properties of polarons in a QR is studied using the methods of the linear-combination operator and the unitary transformation.

2. Theory

For an electron in a QR bounded in a parabolic confined potential with an ellipsoidal boundary condition in different directions x, y, and z, the Hamiltonian of the electron–phonon system in the QR can be written as

$$H = \frac{P_{//}^2}{2m^*} + \frac{P_z^2}{2m^*} + \frac{m^*\omega_0^2\rho^2}{2} + \frac{m^*\omega_z^2 z^2}{2} + \sum_{\boldsymbol{q}} \hbar\omega_{\mathrm{LO}} b_{\boldsymbol{q}}^+ b_{\boldsymbol{q}} + \sum_{\boldsymbol{q}} \left(V_{\boldsymbol{q}} b_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} + h.c.\right), \quad (1)$$

where m^* is the band mass, $\boldsymbol{r} = (x_1, x_2, x_3)$, $x_i (i = 1, 2, 3)$ is the coordinate of an electron, $\rho^2 = x^2 + y^2$, ω_0 and ω_z are the transverse and longitudinal confinement frequencies of the QR, respectively. $b_{\boldsymbol{q}}^+ \left(b_{\boldsymbol{q}}\right)$ is the creation (annihilation) operator of the bulk LO phonons with wave vector $\boldsymbol{q} = (q_{//}, q_z)$.

$$V_{\boldsymbol{q}} = i\left(\frac{\hbar\omega_{\mathrm{LO}}}{q}\right)\left(\frac{\hbar}{2m^*\omega_{\mathrm{LO}}}\right)^{\frac{1}{4}}\left(\frac{4\pi\alpha}{v}\right)^{\frac{1}{2}}, \quad (2)$$

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{\mathrm{LO}}}\right)\left(\frac{2m^*\omega_{\mathrm{LO}}}{\hbar}\right)^{\frac{1}{2}}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \quad (3)$$

where ε_∞ and ε_0 are the static and the high-frequency dielectric constants respectively, α is the electron–LO- phonon coupling strength, and v is the volume of the lattice.

For our cases of QRs, the boundary condition is different from that of spherical QDs. In order to simplify our ellipsoidal

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boundary condition into that of the spherical case, which has a better symmetrical characteristic, we introduce a coordinate transformation that can change the boundary into the spherical one in a new coordinate system[10]. The transformation is $x' = x$, $y' = y$, $z' = z/e'$, where e' is the aspect ratio of the ellipsoid, (x, y, z) are the actual coordinates and (x', y', z') are the transformed ones. Since only the ground-state of the polaron is considered, the effective radius of the ellipsoidal parabolic potential can be introduced[7]: $R_i = \sqrt{\hbar/m^*\omega_i}$, then $R_0 = R_{\rho'} = R_{z'} = R_z/e'$. The Hamiltonian in the new coordinate changes as follows:

$$H = \frac{P_{//}^2}{2m^*} + \frac{e'^2 P_{z'}^2}{2m^*} + \frac{m^*\omega_0^2\rho'^2}{2} + \frac{m^*\omega_{z'}^2 z'^2}{2e'^2} + \sum_{\boldsymbol{q}} \hbar\omega_{\mathrm{LO}} b_{\boldsymbol{q}}^+ b_{\boldsymbol{q}} + \sum_{\boldsymbol{q}} \left(V_{\boldsymbol{q}} b_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}'} + h.c.\right), \tag{4}$$

where $\omega_{z'} = \omega_0$.

We introduce the following first unitary transformation to Eq. (4):

$$U_1 = \exp\left(-i\sum_{\boldsymbol{q}} \boldsymbol{q}\cdot\boldsymbol{r} b_{\boldsymbol{q}}^+ b_{\boldsymbol{q}}\right). \tag{5}$$

We also introduce the linear-combination operators:

$$P_j = \left(\frac{m^*\hbar\lambda}{2}\right)^{\frac{1}{2}} \left(a_j + a_j^+\right), \quad r_j = i\left(\frac{\hbar}{2m^*\lambda}\right)^{\frac{1}{2}} \left(a_j - a_j^+\right), \quad [a_j, a_j^+] = \delta_{ij}, \quad j = x', y', z'. \tag{6}$$

Carrying out a second unitary transformation gives:

$$U_2 = \exp\left(\sum_{\boldsymbol{q}} \left(f_{\boldsymbol{q}} b_{\boldsymbol{q}}^+ - f_{\boldsymbol{q}}^* b_{\boldsymbol{q}}\right)\right). \tag{7}$$

Then the transformed Hamiltonian can be written as

$$H' = U_2^{-1} U_1^{-1} H U_1 U_2. \tag{8}$$

λ is the variational parameter, expressing the polaron's vibrational frequency. $f_{\boldsymbol{q}}$ and $f_{\boldsymbol{q}}^*$ are variational parameters.

We choose the wave-function in the ground state to be

$$|\psi\rangle = \left|\phi(z')\right\rangle \left|0_{\boldsymbol{q}}\right\rangle \left|0_{\mathrm{j}}\right\rangle. \tag{9}$$

$|\phi(z')\rangle$ is the electron's wave-function in the z direction, which satisfies $\langle\phi(z')|\,\phi(z')\rangle = 1$. $\left|0_{\mathrm{q}}\right\rangle$ is the zero-phonon state, and $\left|0_{\mathrm{j}}\right\rangle$ is the vacuum state of the a operator, which satisfied $b_{\boldsymbol{q}}\left|0_{\boldsymbol{q}}\right\rangle = 0$ and $a_{\mathrm{j}}\left|0_{\mathrm{j}}\right\rangle = 0$. The expectation value of Eq. (8) with respect to $|\psi\rangle$ can be expressed as $F\left(\lambda, f_{\boldsymbol{q}}\right) = \langle\psi|\,H'\,|\psi\rangle$. If we choose the usual polaron units ($\hbar = 2m^* = \omega_{\mathrm{LO}} = 1$), using the variational method, we can obtain:

$$\lambda = \frac{2}{R_0^2 e'}\sqrt{\frac{2e'^2+1}{2+e'^2}}, \tag{10}$$

$$E_0 = \begin{cases} \dfrac{1}{R_0^2 e'}\sqrt{(2e'^2+1)(2+e'^2)} - \dfrac{\alpha}{\sqrt{1-e'^2}}\arcsin\sqrt{1-e'^2}, & e' < 1, \\ \dfrac{3}{R_0^2} - \alpha, & e' = 1, \\ \dfrac{1}{R_0^2 e'}\sqrt{(2e'^2+1)(2+e'^2)} - \dfrac{\alpha}{2\sqrt{e'^2-1}}\ln\dfrac{e'+\sqrt{e'^2-1}}{e'-\sqrt{e'^2-1}}, & e' > 1. \end{cases} \tag{11}$$

Equation (10) expresses the vibrational frequency of a polaron, which is related to the effective radius and the electron–LO-phonon coupling strength. Equation (11) is the expression of the ground-state energy. The first item, which expresses the energy of electrons including the kinetic energy and the potential confinement energy, is positive. It depends on the effective radius and the aspect ratio. The second item is negative, which includes the energy of phonons and the interactional electron–phonon energy. It depends on the coupling strength and the aspect ratio.

3. Numerical results and discussion

In the case of a weak electron–LO-phonon coupling, the expressions for the vibrational frequency λ and the ground-state energy E_0 are, respectively, given in Eqs. (10) and (11). In order to distinctly clarify the influences of the effective radius R_0 and the aspect ratio e' on the vibrational frequency and the influences of R_0, e', and coupling strength α on the ground-state energy of a polaron, the numerical results in the usual polaron units are presented in Figs. 1–5.

Figure 1 shows the relationship between λ and R_0 when $e' = 2$. Figure 2 describes the variation of E_0 versus R_0 when $\alpha = 0.1$ and $e' = 2$. From the two figures, we can see that both λ and E_0 increase with decreasing R_0. This is because there is a confining potential that confines the motion of the electrons. As the confining potential ($\omega_0 = \hbar\big/m^* R_0^2$) increases, that is, as r decreases, the thermal motion energy of 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, the vibrational frequency λ and the ground-state energy E_0 of the weak-coupling polaron in a QR both increase. These results show the quantum size effects.

Figure 3 expresses the variation of the vibrational frequency λ versus the aspect ratio e' when $R_0 = 0.4$. From

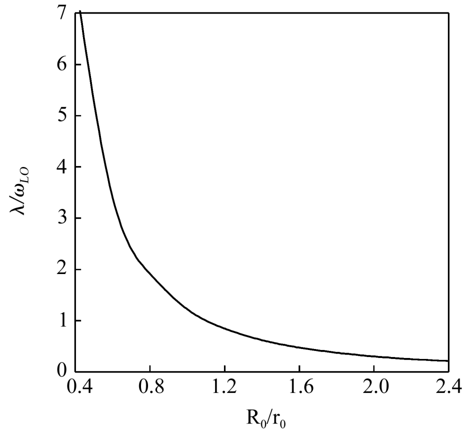

Fig. 1. Relationship of vibration frequency to effective radius R_0 in QR ($e' = 2$) .

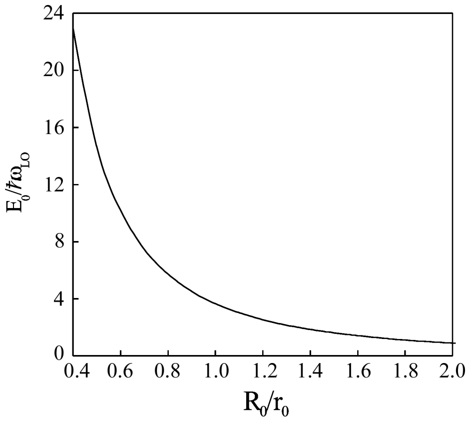

Fig. 2. Relationship of ground-state energy E_0 to effective radius R_0 in QR ($\alpha = 0.1, e' = 2$).

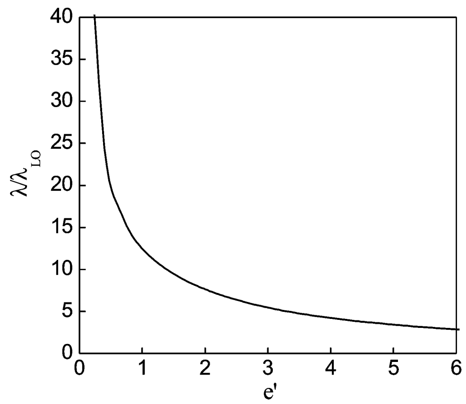

Fig. 3. Relationship of vibration frequency λ to aspect ratio e' in QR ($R_0 = 0.4$).

Fig. 3, λ increases with decreasing e'. Because the decreasing e' leads to a smaller range of particle motion, the vibrational frequency λ will increase, which shows the quantum size effects.

Figure 4 shows the variation of the ground-state energy E_0 versus the aspect ratio e' when $R_0 = 0.4$ and $\alpha = 0.1$. For $0 < e' < 1$, the longitudinal size of the ellipsoid in the QR will decrease with decreasing e', which causes the ground-state energy E_0 to increase. Then, the transverse size of the ellipsoid in the QR equals the longitudinal one when $e' = 1$; accordingly, the ground-state energy E_0 decreases to the minimum. Finally,

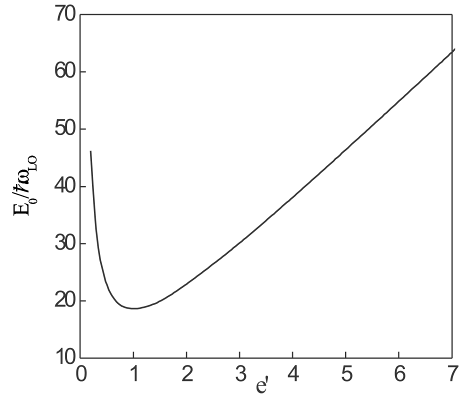

Fig. 4. Relationship of ground-state energy E_0 to aspect ratio e' in QR ($R_0 = 0.4, \alpha = 0.1$).

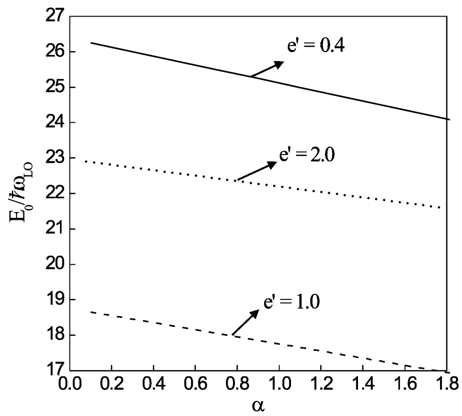

Fig. 5. Relationship of ground-state energy E_0 to coupling strength α and e' in QR ($R_0 = 0.4$).

the transverse size of the ellipsoid in the QR will decrease with increasing e' for $e' > 1$, which causes the ground-state energy E_0 to increase. This shows the interesting quantum size effects.

Figure 5 shows the variation of the ground-state energy E_0 versus the coupling strength α for different aspect ratios e' when $R_0 = 0.4$. It shows that the ground-state energy decreases linearly with an increase of α because increasing the coupling strength leads to an increase of the interactional electron–LO-phonon energy. From Eq. (), we can see that the interactional electron–LO-phonon energy (the second item) is negative. Therefore, the ground-state energy of a polaron in a QR is decreasing. However, compared with the aspect ratio, the values of the coupling strength in the total range have only a slight effect on the ground-state energy.

4. Conclusion

For a weak electron–LO-phonon coupling, using the linear-combination operator and unitary transformation methods, the vibrational frequency and the ground-state energy of weak-coupling polarons are obtained. Numerical results show that the vibrational frequency increases for both a decrease in the effective radius R_0 and the aspect ratio e' of the ellipsoid, and that the ground-state energy increases for both a decrease in the effective radius R_0 and the electron–LO-phonon coupling strength α. In addition, the ground-state energy decreases with e' within $0 < e' < 1$, and reaches a minimum as the aspect ratio is $e' = 1$. It further increases with e' for $e' > 1$.

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