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Influence of the Interaction Between Phonons and Coulomb Potential on the Properties of a Bound Polaron in a Quantum Dot*

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Abstract: The properties of a bound polaron in a parabolic quantum dot with weak electron-LO-phonon coupling under a Coulomb field are studied. The ground state energy of the bound polaron is derived by using a linear combination operator and the perturbation method. The influence of the interaction between phonons with different wave vectors in the recoil process on the ground state energy of the bound polaron is discussed. Numerical calculations are performed, and the results show that the ground state energy increases significantly as the effective confinement length of the quantum dot decreases, considering of the interaction between phonons. When $l_0 > 1.0$, the influence of the interaction between phonons on the ground state energy cannot be ignored.

Key words: parabolic quantum dot; bound polaron; interaction between phonons; ground state energy
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1 Introduction

Recent technological advances in the fabrication of nano-structures have stimulated both experimental and theoretical interest in low-dimensional systems. In recent years, there has been considerable effort to achieve an understanding of the unusual physical properties of quantum dots (QDs) because of their promising application in device engineering. Much theoretical and experimental interest has been devoted to the study of the electronic properties of these zero-dimensional semiconductor systems. The interaction of electrons with LO-phonon in quantum dots has been investigated by many authors[1~4]. Moreover, many investigations have been devoted to the problem of an electron bound to a hydrogenic impurity using different methods. Wang *et al*.[5] investigated the effects of LO phonons on the hydrogen-like impurity in a semiconductor quantum dot. Chen *et al*.[6] derived the expression of the ground-state energy of an electron in parabolic quantum dots and a wire coupled simultaneously with a Coulomb potential and a LO phonon field within the framework of Feynman variational path-integral theory. Melnikov *et al*.[7,8] studied the effect of the electron-phonon interaction on an electron bound to an impurity in a spherical quantum dot embedded in a non-polar matrix. Woggon *et al*.[9] studied the states of polarons bound in a potential and determined the local optical absorption spectrum up to first-order time-dependent perturbation theory with respect to the electron-phonon interaction. Xie *et al*.[10] investigated the binding energy of a bound polaron in a spherical quantum dot by using a variational method. Investigations of the properties of bound polaron in a quantum dot have omitted the interaction between phonons with different wave vectors in the recoil process. The influence of this interaction on the properties of bound polaron in a quantum dot has not been studied so far. In this paper, we study the interaction between phonons on the properties of a bound polaron in a quantum dot by using an integration of the linear combination operator and the perturbation method.

2 Theory

We consider a system in which the electrons are bound by the parabolic potential and Coulomb

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potential. The electrons are much more confined in one direction (taken as the direction z) than in the other two directions (taken as the x-y plane)[11]. Therefore, we shall only consider an electron moving on the x-y plane by taking into account the interaction between the electron and LO-phonons. We assume that the confinement potential in a single QD is parabolic.

$$V_{(\rho)} = \frac{1}{2} m\omega_0^2 \rho^2 \tag{1}$$

The Coulomb bound potential is:

$$V(r) = -\frac{e^2}{\varepsilon_\infty r} \tag{2}$$

where m^* is the band mass of the electron, $r = (\rho, z)$ is the coordinate of the electron, and ω_0 is the confinement strength. The Hamiltonian of the electron-phonon system is given by

$$H = \frac{\hbar^2}{2m}\nabla_\rho^2 + \frac{1}{2}m\omega_0^2\rho^2 + \sum_q \hbar\omega_L a_q^+ a_q + \sum_q (V_q e^{iq\cdot r} a_q + h\cdot c) - \frac{e^2}{\varepsilon_\infty r} \tag{3}$$

where a_q^+ (a_q) is the creation (annihilation) operator of a bulk LO-phonon with wave vector $\boldsymbol{q}$ ($\boldsymbol{q} = q_{/\!/}, q_\perp$),

$$V_q = i(\hbar\omega_{L0}/q)(\hbar/2m\omega_L)^{\frac{1}{4}}(4\pi\alpha/V)^{\frac{1}{2}} \tag{4a}$$

$$\alpha = (e^2/2\hbar\omega_{L0})(2m\omega_L/\hbar)^{\frac{1}{2}}(1/\varepsilon_\infty - 1/\varepsilon_0) \tag{4b}$$

Using the Fourier expansion to the Coulomb bound potential:

$$\frac{1}{r} = \sum_q \frac{4\pi}{Vq^2}\exp(-i\boldsymbol{q}\cdot\boldsymbol{r}) \tag{5}$$

We introduce a linear combination operator and carrying out a unitary transformation

$$p_j = \left(\frac{m\hbar\lambda}{2}\right)^{1/2}(b_j^+ + b_j)$$

$$\rho_j = i\left(\frac{\hbar}{2m\lambda}\right)^{1/2}(b_j - b_j^+), \quad j = x, y \tag{6}$$

$$U_1 = \exp\left(-i\sum_q a_q^+ a_q \hbar\, \boldsymbol{q}\cdot\boldsymbol{r}\right)$$

$$U_2 = \exp\left\{\sum_q (a_q^+ f_q - a_q f_q^*)\right\} \tag{7}$$

The Hamiltonian becomes

$$H' = U_2^{-1}U_1^{-1}HU_1U_2 = H'_0 + H'_1 \tag{8a}$$

Here,

$$H'_1 = \frac{\hbar^2}{2m}\sum_{q\neq q'}(a_{q'}^+ + f_{q'}^*)(a_q + f_q)(a_q + f_q)(a_{q'} + f_{q'})\boldsymbol{q}\cdot\boldsymbol{q}' \tag{8b}$$

Here H'_1 is the attachment energy of the interaction between phonons of different wave vectors in the recoil process.

The ground-state wave function of the system is chosen as

$$|\phi\rangle = |\varphi(z)\rangle|0\rangle|0\rangle_b \tag{9}$$

where $|\varphi(z)\rangle$ is the normalized electron wave function along the z direction and $|\langle\varphi(z)|\varphi(z)\rangle|^2 = \delta(z)$ since the electrons are considered to be confined in an infinitesimally narrow layer. $|0\rangle_b$ is the vacuum state for operator b, and $|0\rangle$ is the unperturbed zero-phonon state.

The expectation value is $F(\lambda, f_q) \equiv \langle\Psi|H'_0|\Psi\rangle$. By using the variational technique to λ, we can obtain f_q and $F(\lambda)$ can be calculated, replacing the summation with an integral.

Using the variational technique, the expression for the vibration frequency of a bound polaron in a quantum dot can be derived as

$$\lambda^2 - \frac{2e^2}{\hbar\varepsilon_\infty}\sqrt{\frac{m}{\pi\hbar}}\lambda^{3/2} - \omega_0^2 = 0 \tag{10a}$$

We have the variational parameter:

$$\lambda = \lambda_0 \tag{10b}$$

The ground state energy of a bound polaron in the weaking-coupling region for electron-phonon interaction can be written as

$$E_{01} = \frac{\hbar\lambda_0}{2} + \frac{\hbar^3}{2l_0^4 m^2\lambda_0} - \alpha\hbar\omega_L - 2\beta\sqrt{\lambda_0} \tag{11}$$

where the effective confinement length is $l_0 = \sqrt{\hbar/m\omega_0}$, and the Coulomb bound potential is $\beta = \frac{e^2}{\varepsilon_\infty}\sqrt{\frac{m}{\pi\hbar}}$. Choosing $\hbar = 2m = \omega_L = 1$ in polaron units, the ground state energy can be written as

$$E_{01} = \frac{\lambda_0}{2} + \frac{2}{l_0^4}\times\frac{1}{\lambda_0} - \alpha - 2\beta\sqrt{\lambda_0} \tag{12}$$

3 Perturbation calculations

We regard H'_0 as the unperturbed Hamiltonian of the system and H'_1 as the perturbation to perform perturbation calculation. The first order perturbation energy is zero and the second order perturbation energy is:

$$\Delta E = -\sum_n{}' \frac{|(H'_1)_{0n}|^2}{E_n - E_0} = -\left(\frac{1}{12} - \frac{2}{9\pi}\right)\alpha^2\hbar\omega_L \tag{13}$$

Considering the second order perturbation energy, the total energy of bound polaron, including the interaction between phonons with different wave vectors in the recoil process, can be written as

$$E_0 = E_{01} + \Delta E = \frac{\hbar\lambda_0}{2} + \frac{\hbar^3}{2l_0^4 m^2\lambda_0} - \alpha\hbar\omega_L - 2\beta\sqrt{\lambda_0} - \left(\frac{1}{12} - \frac{2}{9\pi}\right)\alpha^2\hbar\omega_L \tag{14}$$

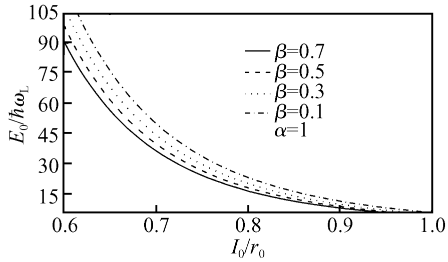

Fig.1　Relational curves of the ground state energy E_0 and the effective confinement length l_0 at different Coulomb bound potentials β

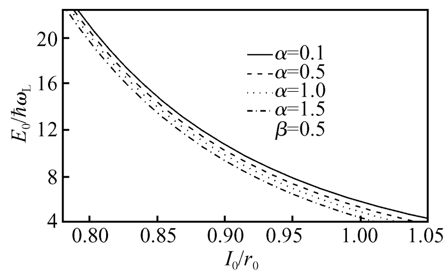

Fig.2　Relational curves of the ground state energy E_0 and the effective confinement length l_0 at different electron-LO-phonon coupling strengths α

Choosing $\hbar = 2m = \omega_L = 1$ in polaron units，we obtain：

$$E_0 = \frac{\lambda_0}{2} + \frac{2}{l_0^4\lambda_0} - \alpha - 2\beta\sqrt{\lambda_0} - \left(\frac{1}{12} - \frac{2}{9\pi}\right)\alpha^2 \tag{15}$$

4　Numerical results and discussion

Considering the interaction between phonons of different wave vectors in the recoil process, the ground state energy of bound polaron in a parabolic QD is not only related to the effective confinement length l_0, the electron-LO-phonon coupling strength α, and the Coulomb bound potential β, but also related to the interaction between phonons. The numerical results of the dependence of the ground-state energy on the confinement length, the electron-LO-phonon coupling strength, the Coulomb bound potential and the interaction between phonons are presented in Figs. 1 to 5 (chosen $\hbar = 2m = \omega_L$ in polaron units).

Figures 1 and 2 show the ground state energy as a function of the effective confinement length l_0 for different the electron-LO-phonon coupling strengths and Coulomb bound potentials. The ground state energy increases rapidly as the confinement length decreases. Furthermore, the ground state energy also increases rapidly as the effective confinement length decreases when considering the interaction between phonons of different wave vectors in the recoil process since there is a confinement potential to confine the motion of the electrons. As the confinement length decreases (ω_0 increases), that is, as r decreases, the thermal motion energy of electrons and the interaction between electron and phonons, which take phonons as medium, is enhanced because the range of the particles' motion becomes small. As a result, the ground-state energy increases due to quantum size effects. Figure 1 shows that, holding confinement length constant, the smaller the Coulomb bound potential is, the higher the ground state energy is. Figure 2 shows that, holding confinement length constant, the smaller the electron-LO-phonon coupling strength is, the higher the ground state energy is.

Considering the interaction between phonons of different wave vectors in the recoil process, the corresponding energy of bound polaron is $E_{01} - E_0$ and the ground state energy is E_0. To obtain the relationship between the corresponding energy and the total energy, we have：

$$P = \frac{E_{01} - E_0}{E_0} = \frac{\left(\frac{1}{12} - \frac{2}{9\pi}\right)\alpha^2}{\frac{\lambda_0}{2} + \frac{2}{l_0^4\lambda_0} - \alpha - 2\beta\sqrt{\lambda_0} - \left(\frac{1}{12} - \frac{2}{9\pi}\right)\alpha^2} \tag{16}$$

The value of P is the ratio of the interaction energy between phonons of different wave vectors in the recoil process and the total energy. Equation (16) indicates that the value of P is not only related to the electron-LO-phonon coupling strength α and the Coulomb bound potential β, but also to the effective confinement length. Figures 3 and 4 show the value of P as a function of the effective confinement length l_0 for different electron-LO-phonon coupling strengths and Coulomb bound potentials. Figures 3 and 4 demonstrate that the value of P increases as the effective confinement length l_0 increases. Holding confinement length constant, the bigger the Coulomb bound potential and electron-LO-phonon coupling strength are, the higher the value of P is.

Figure 5 shows the value of P as a function of the effective confinement length l_0. We can see

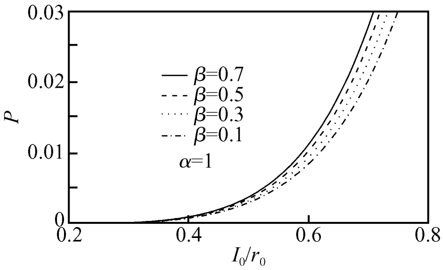

Fig.3 Relational curves of P and the effective confinement length l_0 at different Coulomb bound potentials β

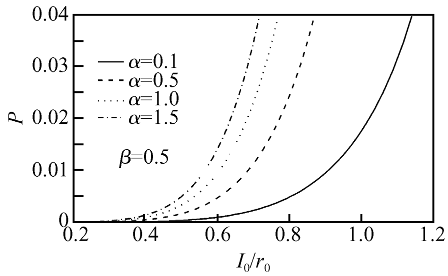

Fig.4 Relational curves of P and the effective confinement length l_0 at different electron-LO-phonon coupling strengths α

that the value of P and the change rate of the effective confinement length l_0 are small when $l_0 < 1.0$. This is because the influence of the Coulomb potential and confine potential on the ground state energy is much greater than the influence of the interaction between phonons on it. However, the value of P increases rapidly as the effective confinement length l_0 increases when $l_0 > 1.0$. Figures 1 and 2 indicate that, holding confinement length constant, the smaller the electron-LO-phonon coupling strength and the smaller Coulomb bound potential are, the higher the ground state energy is. The third, the forth and the fifth terms in Eq.(15) are negative whereas the total energy is positive. The influence of Coulomb potential and confine potential on the ground state energy is much smaller than the influence of the interaction between phonons on it. Therefore, the influence of the interaction between phonons on the ground state energy must be considered when one discusses the problem of bound polarons in QDs.

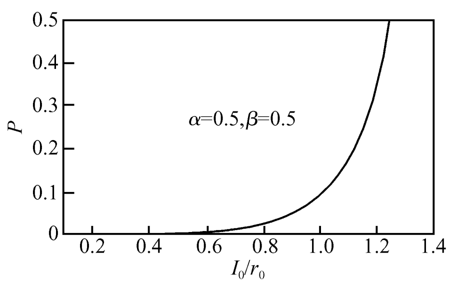

Fig.5 Relational curve of P and the effective confinement length l_0

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声子之间相互作用和库仑势对量子点中束缚极化子性质的影响*

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摘要：研究了库仑场中抛物量子点中束缚极化子的性质.采用线性组合算符和微扰法，导出了量子点中束缚极化子的基态能量.在计及电子在反冲效应中发射和吸收不同波矢的声子之间的相互作用下，研究了其对量子点中束缚极化子的基态能量的影响.数值计算表明：当考虑声子之间的相互作用时，量子点中束缚极化子的基态能量随量子点的有效受限长度的减小而迅速增大.当 $l_0>1.0$ 时，必须考虑声子之间的相互作用对基态能量的影响.

关键词：抛物量子点；束缚极化子；声子之间相互作用；基态能量
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