Influence of Coulomb Potential on the Properties of a Polaron in a Quantum Dot*

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Abstract: The ground-state energy and the average number of virtual phonons around the electron of a hydrogenic impurity confined in a parabolic quantum dot are calculated using the squeezed-state variational approach, which is based on two successive canonical transformations and uses a displaced-oscillator type unitary transformation to deal with the bilinear terms, which are usually neglected. Numerical calculations are carried out in order to study the relation between the ground-state energy and the average number of virtual phonons around the electron of a bound polaron in a parabolic quantum dot with the Coulomb binding parameter. The electron-phonon coupling constant and the confinement length are derived.

Key words: squeezed-state; quantum dot; polaron
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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. During recent decades, great progress in epitaxial crystal growth techniques has made it possible to fabricate quasi-zero-dimensional (Q0D) structures, with very low background impurity concentrations. This has led to much intensive study on these low-dimensional systems because of their potential device applications. Due to the reduction of the dimensionality of systems from 3D to Q0D, electron-phonon interactions have more pronounced effects than in bulk materials. The interaction of an electron with an LO-phonon in such quantum dots has been investigated by many authors[1,2]. Moreover, many investigations have been devoted to the problem of an electron bound to a hydrogenic impurity using various methods[3].

A recent work[4] studied the polaronic correction to the ground- and the first-excited state energy of an electron interacting with optical-phonons by a variational approach with a squeezed-state. Another recent work[5] studied the ground-state binding energy of an impurity magnetopolaron in a parabolic quantum dot (QD) using the squeezed-state variational approach. However, there have been few investigations on the properties of a bound polaron in a parabolic QD by using the squeezed-state variational approach.

In this paper, the unitary transformation scheme is developed to diagonalize the well-known Hamiltonian describing an impurity polaron confined in a 3D parabolic QD. Our variational approach is based on two successive canonical transformations. One is a displaced-oscillator type unitary transformation to diagonalize the relevant Fröhlich Hamiltonian, and the other is a single-mode squeezed-state transformation, which is used to deal with the bilinear terms of phonon creation and annihilation operators arising from the first transformation. The ground-state energy and the average number of virtual phonons around the electron of weak- and strong-coupling bound polarons in a QD with a parabolic Coulomb bounding potential are calculated.

2 Theory

We assume the confining potential in a single QD is parabolic $V(\boldsymbol{r}) = m^* \omega_0^2 \boldsymbol{r}^2/2$ with the Coulomb bounding potential $V(\boldsymbol{r}) = -e^2/\varepsilon_\infty r^2$, where

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m^* is the bare band mass, $\boldsymbol{r}$ is the coordinate vector of the three-dimensional QD, p is the moment operator of the electron, and ω_0 is the confinement strength of the QD. An impurity polaron in a 3D parabolic QD potential is described by the Fröhlich Hamiltonian.

$$H = H_{\mathrm{E}} + \sum_{q} \hbar\omega_{\mathrm{L0}} b_q^+ b_q + \sum_{q} (V_q b_q \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} + h \cdot c) \quad (1)$$

$$H_{\mathrm{E}} = \frac{1}{2m^*} p^2 - \frac{e^2}{\varepsilon_\infty r} + \frac{1}{2} m^* \omega_0^2 \boldsymbol{r}^2 \quad (2)$$

Here b_q^+ (b_q) is the creation (annihilation) operator of an optical phonon, and

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

$$\alpha = (e^2/2\hbar\omega_{\mathrm{L0}})(2m^*\omega_{\mathrm{L0}}/\hbar)^{\frac{1}{2}}(1/\varepsilon_\infty - 1/\varepsilon_0)$$

The phonon displacement is given by $F_q(\boldsymbol{r}) = f_q \exp[-\mathrm{i}(1-\lambda)\boldsymbol{q}\cdot\boldsymbol{r}]$. The first step is to carry out a unitary transformation of displaced-oscillator type:

$$U_1 = \exp\left\{\sum_q [F_q^*(\boldsymbol{r}) b_q - F_q(\boldsymbol{r}) b_q^+]\right\} \quad (3)$$

After diagonalizing the phonon-related part of the Hamiltonian, we can easily obtain $\tilde{H} = U_1^{-1} H U_1 = H_{\mathrm{E}} + H_0 + H_1 + H_2$, each term of which is respectively given by

$$H_0 = \sum_q \left[\frac{\hbar^2}{2m^*} |\nabla F_q(\boldsymbol{r})|^2 + \hbar\omega_{\mathrm{L0}} |\nabla F_q(\boldsymbol{r})|^2 - V_q F_q(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} - h \cdot c\right]$$

$$H_1 = \sum_q \hbar\omega_{\mathrm{L0}} b_q^+ b_q + \sum_q \left\{\left[V_q^* \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} + \frac{\hbar^2}{\mathrm{i}m^*}\boldsymbol{p}\cdot\nabla F_q(\boldsymbol{r}) - \hbar\omega_{\mathrm{L0}} F_q(\boldsymbol{r})\right] b_q^+ + h \cdot c\right\}$$

$$H_2 = \sum_q \sum_{q'} \frac{\hbar^2}{2m^*} [2\nabla F_q(\boldsymbol{r}) \cdot \nabla F_{q'}^*(\boldsymbol{r}) b_q^+ b_{q'} - \nabla F_q(\boldsymbol{r}) \cdot \nabla F_{q'}(\boldsymbol{r}) b_q^+ b_{q'}^+ - \nabla F_q^*(\boldsymbol{r}) \cdot \nabla F_{q'}^*(\boldsymbol{r}) b_q b_{q'}] \quad (4)$$

The second step is to introduce the single-mode squeezed-state transformation:

$$U_2 = \exp\left\{\frac{1}{2}\sum_q G_q [(b_q^+)^2 - (b_q)^2]\right\} \quad (5)$$

After the second transformation under U_2, H_1 and H_2 are straightforward, and the non-vanishing contribution to H_0 is found to be $\tilde{H}_2$, using the Fourier expansion $\frac{1}{\boldsymbol{r}} = \frac{4\pi}{V}\sum_q \frac{1}{q^2}\exp(-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r})$[6,7]. We then have

$$\tilde{H}_2 = \sum_q \left\{\left[\hbar\omega_{\mathrm{L0}} + \frac{\hbar^2}{m^*} |\nabla F_q(\boldsymbol{r})|^2\right]\sinh^2 G_q - \frac{\hbar^2}{2m^*}[\nabla F_q(r) \nabla F_q(\boldsymbol{r}) + \nabla F_q^*(\boldsymbol{r}) \nabla F_q^*(\boldsymbol{r})]\sinh G_q \cosh G_q \quad (6)$$

The final Hamiltonian is $\tilde{H}' = H_{\mathrm{E}} + H_0 + \tilde{H}_2$.

We choose the trial wave-function in the ground-state by the variational method of Pekar type to be $|\Psi\rangle = |r\rangle \otimes |0\rangle_{\mathrm{PH}}$, where $|0\rangle_{\mathrm{PH}}$ is the phonon vacuum state. The electron part of the trial wave-function is now written as

$$\Phi(r) = \left(\frac{\gamma}{\sqrt{\pi}}\right)^{\frac{3}{2}} \exp[-\gamma^2 r^2/2] \quad (7)$$

By minimizing the expectation value of the Hamiltonian, that is $E_0 = \langle\Psi|\tilde{H}'|\Psi\rangle$, we obtain

$$E(\gamma) = \frac{3}{4m^*}\gamma^2 + \frac{3}{4\gamma^2} m^* \omega_0^2 + \frac{2}{\sqrt{\pi}}\beta\gamma + \sum_q \left\{\left[\hbar\omega_{\mathrm{L0}} + \frac{\hbar^2 q^2}{2m^*}(1-\lambda)^2\right]|f_q|^2 - V_q f_q \sigma(\lambda\boldsymbol{q}) - V_q^* f_q^* \sigma(\lambda\boldsymbol{q})\right\} + \sum_q \left\{\left[\hbar\omega_{\mathrm{L0}} + \frac{\hbar^2 q^2}{m^*}(1-\lambda)^2 |f_q|^2\right]\sinh^2 G_q + \frac{\hbar^2 q^2}{2m^*}(1-\lambda)^2 \sigma[2(1-\lambda)\boldsymbol{q}](f_q^2 + f_q^{*2})\sinh G_q \cosh G_q\right\} \quad (8)$$

where $\beta = \frac{e^2}{\varepsilon_\infty}\sqrt{\frac{m^*}{\pi\hbar}}$ is the Coulomb binding parameter and $\sigma(\lambda q) = \langle\exp(\mathrm{i}\lambda\boldsymbol{q}\cdot\boldsymbol{r})\rangle$, $\langle\cdots\rangle$ denotes the expectation value with respect to electronic coordinates, and $\lambda = 1$ and $\lambda = 0$ are equivalent to the results of the strong- and weak-coupling regimes:

$$H_q = \hbar\omega_{\mathrm{L0}} + \frac{\hbar^2 q^2}{m^*}(1-\lambda)^2 |f_q|^2$$

$$J_q = \frac{\hbar^2 q^2}{2m^*}(1-\lambda)^2 \sigma[2(1-\lambda)\boldsymbol{q}](f_q^2 + f_q^{*2}) \quad (9)$$

After inserting Eq. (9) into Eq. (8), we obtain f_q and G_q by using the variational techniques,

$$f_q = \frac{V_q}{\hbar\omega_{\mathrm{L0}} + \frac{\hbar^2 q^2 (1-\lambda)^2}{2m^*} F(\boldsymbol{q}, \lambda; G_q)} \sigma(\lambda\boldsymbol{q})$$

$$G_q = \frac{1}{2}\tanh^{-1} J_q/H_q \quad (10)$$

where $F(\boldsymbol{q}, \lambda; G_q) = \cosh 2G_q - \sigma(2\lambda\boldsymbol{q})\sinh 2G_q$.

3 Results and discussion

We comment on a particular form of Eq. (8), in the limit of vanishing G_q and obtain $F(q, \lambda; 0)$. Using the variational techniques, we have the variational parameter $\gamma = \gamma_0$. Choosing in the usual polaron units $\hbar = 2m^* = \omega_{\mathrm{L0}} = 1$ and $l_0 = \sqrt{\hbar/m^*\omega_0}$ which is the effective confinement

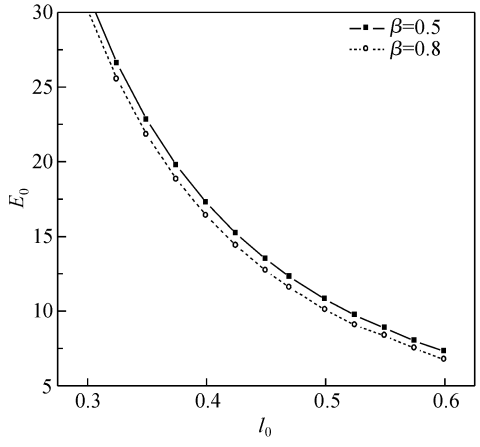

Fig. 1　Weak-coupling bound polaron ground-state energy E_0 in a parabolic quantum dot as a function of the confinement length l_0 for $\alpha = 0.5, \beta = 0.5$ and 0.8

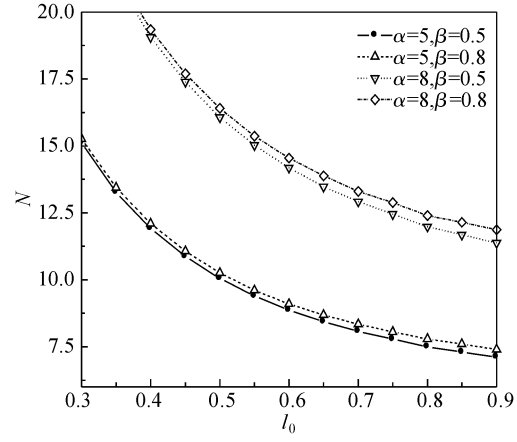

Fig. 3　Average number of virtual phonons N around the electron in the ground-state in a parabolic quantum dot as a function of the confinement length for $\alpha = 5$ and $8, \beta = 0.5$ and 0.8 of strong-coupling limit

length, the ground-state energy E_0 can be easily obtained. The average number of virtual phonons around the electron is easily calculated as

$$N = \langle \Psi \mid U_2^{-1} U_1^{-1} \sum_q b_q^+ b_q U_1 U_2 \mid \Psi \rangle = \begin{cases} \alpha, & \lambda = 0 \\ \sqrt{\dfrac{2}{\pi}} \alpha \gamma_0, & \lambda = 1 \end{cases} \tag{11}$$

The numerical results of the dependence of the ground-state energy and the average number of virtual phonons around the electron on the confinement length, the electron-LO-phonon coupling constant, and the Coulomb binding parameter are presented in Fig. 1 to Fig. 3.

Figure 1 shows the ground-state energy of a bound polaron in the electron-LO-phonon weak-coupling case as a function of the confinement l_0 for $\alpha = 0.5, \beta = 0.5$ and 0.8. From it we can see that the ground-state energy increases rapidly as the confinement length decreases. This result is in agreement with the results of Chen *et al*.[8], which is obtained by using the Feynman-Haken path-integral approach, and of Chen[9], which is obtained by using the linear combination operator and unitary transformation methods. We also see that at the same value of confinement length, the larger Coulomb binding parameter β is, the smaller the ground-state energy is. Figure 2 displays the ground-state energy of the bound polaron versus the confinement length for $\alpha = 5, \beta = 0.5$ and 0.8 in the electron-LO-phonon strong-coupling case. From Fig. 2, it can be seen that the ground-state energy increases with decreasing confinement length. This result is in agreement with the result of Chen *et al*.[10], which was obtained by using the variational path integral theory. At the same confinement length, the larger the Coulomb binding parameter β is, the smaller is the ground-state energy. Figure 3 presents the average number of virtual phonons around the electron as a function of the confinement length for different electron-LO-phonon coupling constants and different values of the Coulomb binding parameter β in the electron-LO-phonon strong-coupling case. It is shown that the average number of virtual phonons around the electron decreases with increasing confinement length. The result is in agreement with the result of Wang *et al*.[11], which is obtained by

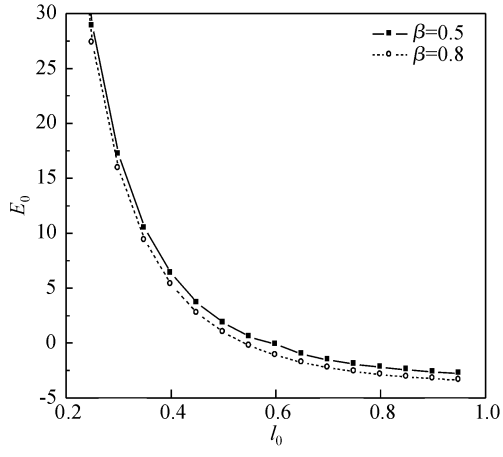

Fig. 2　Strong-coupling bound polaron ground-state energy E_0 in a parabolic quantum dot as a function of the confinement length l_0 for $\alpha = 5, \beta = 0.5$ and 0.8

using the linear combination operator and unitary transformation methods. At the same value of confinement length and the same value of electron-LO-phonon coupling constant, the larger the Coulomb binding parameter β is, the larger is the average number of virtual phonons around the electron. At the same values of confinement length and Coulomb binding parameter β, the larger the electron-LO-phonon coupling constant is, the larger is the average number of virtual phonons around the electron. The average number N is a fixed value when the electron-LO-phonon coupling constant α is fixed, and it is independent of the other parameters according to Eq. (11) within the range of electron-phonon weak-coupling. The thermal motion energy which takes phonons as a medium and the interaction between the electron and phonons become more intense with decreasing confinement length (increasing ω_0), that is, with decreasing r. This is because the range of the particle's motion becomes smaller. As a result, the ground-state energy and the average number of phonons of the bound polaron all increase. This is attributed to interesting quantum size effects. For a given confining potential, the larger the electron-LO-phonon coupling strength is, the larger are the ground-state energy and the average number of phonons of the bound polaron. Then the polarization of the quantum dot is strengthened. From what has been discussed above, it is clear that the polarization of the quantum dot cannot be omitted. These results indicate that our method agrees with other methods and the ground-state energy and the average number of virtual phonons both have corrections considering the effects of the quadratic terms. It is shown that the effects of the quadratic terms that we have often omitted are very important and should be taken into account in researching the size-dependent physical properties of nano-structured materials.

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库仑场对量子点中极化子性质的影响*

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摘要：采用基于逐次正则变换的变分方法，利用单模压缩态变换处理包含声子产生湮灭算符的双线性项，研究了抛物量子点中束缚极化子的性质.得到了在电子-体纵光学声子强、弱耦合极限下抛物量子点束缚极化子的基态能量及电子周围平均声子数.讨论了受限长度，电子-体纵光学声子耦合常数，库仑结合参数与基态能量和平均声子数之间的依赖关系.

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