The energy levels of a two-electron two-dimensional parabolic quantum dot*

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This paper studies the two-electron total energy and the energy of the electron–electron interaction by using a variational method of Pekar type on the condition of electric–LO-phonon strong coupling in a parabolic quantum dot. It considers the following three cases: 1) two electrons are in the ground state; 2) one electron is in the ground state, the other is in the first-excited state; 3) two electrons are in the first-excited state. The relations of the two-electron total energy and the energy of the electron–electron interaction on the Coulomb binding parameter, the electron-LO-phonon coupling constant and the confinement length of the quantum dot are derived in the three cases.

Keywords: quantum dot, electron–electron interaction, the variational method of Pekar type

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1. Introduction

During the past decade, much attention has been paid to quantum dots (QDs),[1,2] in which only a few electrons are bound in semiconductor heterostructures. Essentially, they are little islands of two-dimensional (2D) electrons, which are laterally confined by an artificial potential. Alternatively, they can be considered as artificial atoms where a confining potential replaces the potential of the nucleus. Therefore, these atomic-like few-electron systems can be called artificial atoms as well, in comparison with natural atoms whose electrons move in a spherical central field including the averaged contribution from the electron–electron interaction. Experimentally, QDs have been studied by vertical tunnelling,[3] in-plane transport,[4] capacitance versus voltage curves,[5,6] as well as far-infrared spectroscopy.[7] Theoretically, the exact diagonalization,[8,9] Hartree,[10] and Hartree–Fock methods[11] were used in the early development of QD theory. More recent approaches, including the dimensional perturbation theory,[12] the spin density function theory,[13] the quantum Monte Carlo method,[14,15] and the effective mass theory,[16−19] were proposed with goals including correlation and maintaining accuracy for many-electron dots while simultaneously reducing computational expense. Yannouleas and Landman[20] have investigated the rovibrational spectrum of a two-electron (2e) 2D parabolic QD. Sun and Dong[21,22] have studied the energy spectra and electronic structure of a 2e QD within the effective mass theory. In this article, we study the 2e total energy and the energy of the electron–electron interaction by using a variational method of Pekar type on the condition of electric–LO-phonon strong coupling in a parabolic QD. We consider the following three cases: 1) two electrons are in the ground state; 2) one electron is in the ground state, the other is in the first-excited state; 3) two electrons are in the first-excited state. Numerical calculations are performed and the results illustrate that when the electron–LO-phonon coupling constant increases, the 2e total energy E_{00} increases, the 2e total energies E_{01}, E_{11} decrease and then increase but they decrease as the confinement length of QD and the Coulomb binding parameter increases. The energies of the electron–electron interaction decrease when the Coulomb binding parameter and the confinement length increase but they increase as the electron–LO-phonon coupling constant increases. Our results should be meaningful for investigating the properties of many electrons in QD both theoretically and experimentally.

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2. Theoretical model

We consider two electrons, each with an effective mass m^* at the $z = 0$ plane in a 2e 2D QD, in which the electrons are bounded by the parabolic potential. The electrons are much more confined in one direction (taken as the Z direction) than in the other two directions. Therefore, we shall confine ourselves to considering only the effect of the electron and LO-phonon and only the electron moving on the X–Y plane. We assume that the confining potential in a single QD is parabolic.

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

where the 2D coordinate vector is ρ and ω_0 is the confinement strength, the confinement length of a QD is defined as $l_0 = (\hbar/m^*\omega_0)^{1/2}$. The Hamiltonian of the 2e 2D QD can be written as follows:

$$H = \sum_{n=1}^{2} \left[-\frac{\hbar^2}{2m^*}\nabla_n^2 + \frac{1}{2} m^* \omega_0^2 \rho_n^2 + \sum_{q_n} \hbar\omega_{\rm LO} b_{q_n}^{\dagger} b_{q_n} + \sum_{q_n} (V_{q_n} \mathrm{e}^{\mathrm{i}q_n \cdot \rho_n} b_{q_n} + \text{h.c.}) \right] + \frac{\beta}{|\rho_1 - \rho_2|}, \tag{2}$$

where $b_{q_n}^{\dagger}(b_{q_n})$ is the creation (annihilation) operator of a bulk LO-phonon with the wave vector q_n ($q_n = q_{\parallel}, q_{\perp}$), $\beta = e^2/4\pi\varepsilon_0$ is the Coulomb binding parameter

$$V_{q_n} = \mathrm{i}(\hbar\omega_{\rm LO}/q_n)(\hbar/2m^*\omega_{\rm LO})^{1/4}(4\pi\alpha/V)^{1/2}, \tag{3}$$

$$\alpha = (e^2/2\hbar\omega_{\rm LO})(2m^*\omega_{\rm LO}/\hbar)^{1/2}(1/\varepsilon_{\infty} - 1/\varepsilon_0). \tag{4}$$

Using the Lee–Low–Pines transformation for Eq. (2)

$$U = \left[\exp \sum_{q_n} (f_{q_n} b_{q_n}^{\dagger} - f_{q_n}^* b_{q_n}) \right], \tag{5}$$

where f_{q_n} will be treated as a variational function, we have

$$H' = U^{-1} H U. \tag{6}$$

Suppose that the Gaussian function approximation of a single electron is valid in the ground-state and the first-excited state of the system by a variational method of Pekar type[23]

$$\left|\varphi_n^{(0)}\right\rangle = \frac{\lambda_n}{\sqrt{\pi}} \exp\left(-\frac{\lambda_n^2 \rho_n^2}{2}\right) |\xi(z)\rangle\, |0_{q_n}\rangle \quad (n = 1, 2), \tag{7}$$

$$\left|\varphi_m^{(1)}\right\rangle = \frac{\lambda_m^2}{\sqrt{\pi}} \rho_m \exp\left(-\frac{\lambda_m^2 \rho_m^2}{2}\right) |\xi(z)\rangle\, |0_{q_m}\rangle \, (m = 1, 2), \tag{8}$$

where λ_n, λ_m are the variational parameters, since the electrons are much more strongly confined in the Z direction than in the other two directions and is considered to be confined in an infinitesimally narrow layer, so $\langle\xi(z)|\,\xi(z)\rangle = \delta(z)$. $|0_{q_n}\rangle$ is an unperturbed zero phonon state which satisfies $b_{q_n}|0_{q_n}\rangle = 0$. We then obtain the 2e total energy and the energy of the electron–electron interaction as follows:

$$E_{jj'} = \left\langle \psi^{(jj')} \right| H' \left| \psi^{(jj')} \right\rangle \quad (j, j' = 0, 1), \tag{9}$$

where the two-electron wave function is $\left\langle \psi^{(jj')} \right| = \left\langle \varphi_n^j \right| \left\langle \varphi_m^{j'} \right|$ $(m, n = 1, 2, m \neq n), (j, j' = 0, 1)$.

3. Results and discussion

The numerical results of the 2e total energy and the energy of the electron–electron interaction versus the Coulomb binding parameter, the electron–LO-phonon coupling constant and the confinement length in a parabolic QD are presented in the following figures. Throughout this study, the polaron radius $r_0 = (\hbar/2m^*\omega_{\rm LO})^{1/2}$ and the phonon energy constant $R^* = \hbar\omega_{\rm LO}$ are taken to be the length and energy units respectively.

Figure 1 presents the 2e total energy and the energy of the electron–electron interaction as a function of the electron–LO-phonon coupling constant for the Coulomb binding parameter $\beta = 2$, the confinement length $l_0 = 0.5r_0$. From Fig. 1, it can be seen that when the electron–LO-phonon coupling constant increases, the 2e total energy E_{00} increases, the 2e total energies E_{01}, E_{11} decrease and then increase, but the energies of the electron–electron interaction increase in three cases. So the influence of the energy of the electron–electron interaction on the two-electron total energy is very small. Meanwhile, we also see that the energy of the electron–electron interaction is the largest when two electrons are in the ground state; the smallest is when two electrons are in the first-excited state.

Figure 2 shows the 2e total energy and the energy of the electron–electron interaction as a function of the confinement length of QD for the Coulomb binding parameter $\beta = 2$, the electron–LO-phonon coupling constant

$\alpha = 6$. It shows that the 2e total energy decreases quickly as the confinement length increases. The reason is that when the confinement length increases, the thermal motion energy of electrons and the interaction between electron and phonons, which takes the phonon as the medium, are reduced because the range of motion of electrons becomes large. This is also because the electron motion scope expands with the increase of confinement length. The distance between two electrons also increases due to the increase of confinement length, consequently the energy of the electron–electron interaction decreases.

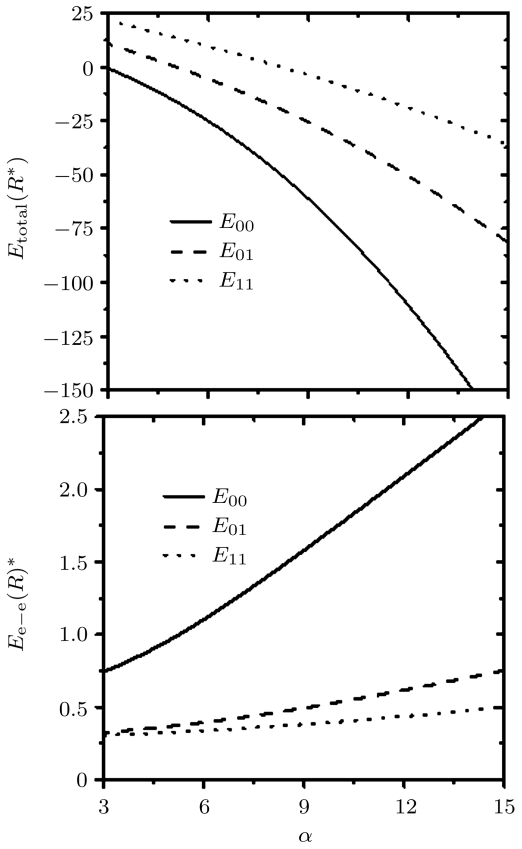


Fig. 1. The two-electron total energy and the energy of the electron–electron interaction as a function of the electron–LO-phonon coupling constant.

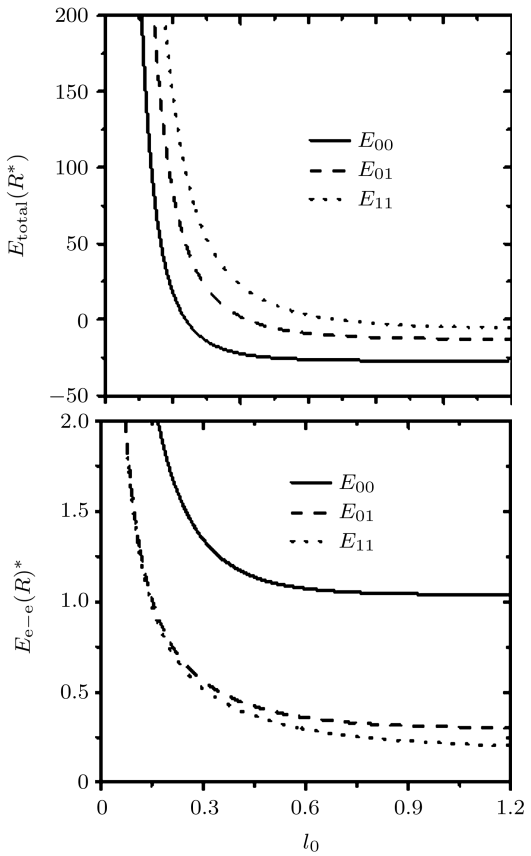


Fig. 2. The two-electron total energy and the energy of the electron–electron interaction as a function of the confinement length.

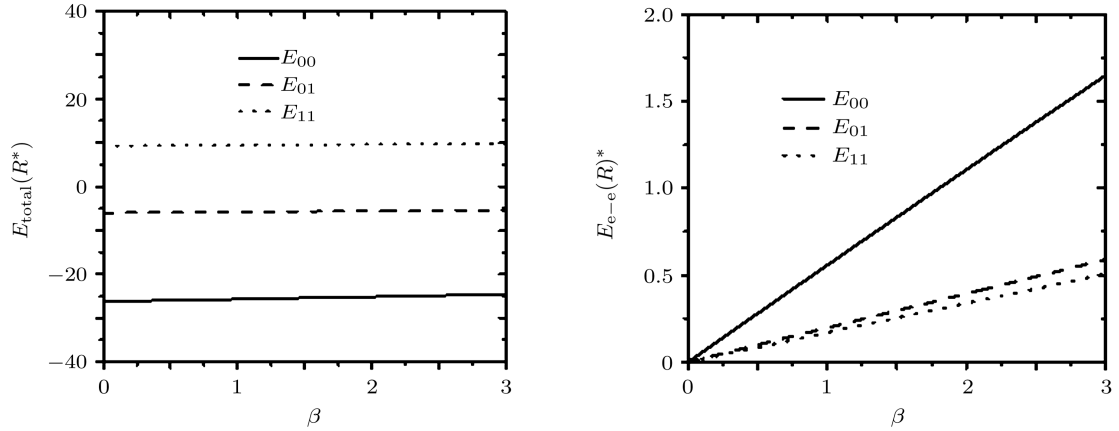


Fig. 3. The two-electron total energy and the energy of the electron–electron interaction as a function of the Coulomb binding parameter.

Figure 3 plots the 2e total energy and the energy of the electron–electron interaction as a function of the

Coulomb binding parameter for the confinement length of QD $l_0 = 0.5r_0$, the electron–LO-phonon coupling constant $\alpha = 6$. It is seen that the 2e total energy decreases and the energy of the electron–electron interaction increases with the increase of the Coulomb binding parameter which is related to the material of QD.

4. Conclusion

Under the condition of strong electron–LO-phonon coupling by using a variational method of Pekar type in a parabolic quantum dot, we studied the 2e total energy and the energy of the electron–electron interaction. The following three cases are considered: 1) two electrons are in the ground state; 2) one electron is in the ground state, the other is in the first-excited state; 3) two electrons are in the first-excited state. The results illustrate that when the electron–LO-phonon coupling constant increases, the two-electron total energy E_{00} increases, the 2e total energies E_{01}, E_{11} decrease and then increase, and they decrease as the confinement length of QD and the Coulomb binding parameter increase. The energies of the electron–electron interaction decrease when the Coulomb binding parameter and the confinement length increase but they increase as the electron–LO-phonon coupling constant increases.

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