Properties of strong-coupling magneto-bipolaron qubit in quantum dot under magnetic field*

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Based on the variational method of Pekar type, we study the energies and the wave-functions of the ground and the first-excited states of magneto-bipolaron, which is strongly coupled to the LO phonon in a parabolic potential quantum dot under an applied magnetic field, thus built up a quantum dot magneto-bipolaron qubit. The results show that the oscillation period of the probability density of the two electrons in the qubit decreases with increasing electron–phonon coupling strength α, resonant frequency of the magnetic field ω_c, confinement strength of the quantum dot ω_0, and dielectric constant ratio of the medium η; the probability density of the two electrons in the qubit oscillates periodically with increasing time t, angular coordinate φ_2, and dielectric constant ratio of the medium η; the probability of electron appearing near the center of the quantum dot is larger, and the probability of electron appearing away from the center of the quantum dot is much smaller.

Keywords: quantum dot, magneto-bipolaron, qubit, Lee–Low–Pines–Pekar variational method

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1. Introduction

Since Feynman[1,2] put forward the concept of quantum computer following the quantum mechanics laws in 1980s, researchers started to study theoretically and experimentally the quantum computer (QC), and QC gradually became a hot spot of information science. The basic information storage and process unit of QC is qubit. Many two-state quantum systems can be used as the carrier of qubit.[3–6] People have proposed various solutions to obtain qubit. At present, the solutions which have made some progresses include the cavity quantum electrodynamics, the ion trap, the liquid-state nuclear magnetic resonance, etc.[7–10] However, the common disadvantage of these solutions is unable to obtain a large number of qubits. To achieve the large scale integration of qubits, we have to adopt a solid-state qubit system. This system is easier to achieve miniaturization and integration of a large number of qubits, and it has more potential to manufacture a truly practical QC, thus, many researchers start to study the quantum dot qubit and have obtained a series of important results.[11–14]

In recent years, many researchers studied the effect of the electron–phonon interaction on qubit in quantum dot.[15–18] Most of those studies are limited to discuss the qubit structured by the monopolaron ground state and the first excited state, and there is no doubt that it is correct for the III–V semiconductor quantum dot. However, with the development of the semiconductor material growth technology, the I–VII semiconductors (such as RbCl, KI, etc.) have drawn much attention in recent years. As the electron–phonon coupling constant of the I–VII semiconductors is an order of magnitude larger than that of the III–V semiconductors, and the electron–phonon interaction in the quantum dot made of such materials becomes even stronger due to the lower dimensionality (usually the electron–phonon coupling strength is greater than 6), the bound state of bipolaron can be formed by the interaction between two identical electrons through the phonon field.[19–21] In the study of bipolaron in magnetic field, one of the authors[21] first proposed the concept of magneto-bipolaron. It is no doubt that, for the quantum dot made of I–VII semiconductor materials, it is impossible and not necessary to restrain the bipolaron formation, and the study of the bipolaron qubit has more practical significance and potential in application than the study of the polaron qubit alone. We adopt the variational method of the Pekar type based on the Lee–Low–Pines (LLP) unitary transformation and study the property of the qubit structured by the strong-coupling magneto-bipolaron ground state and the first excited state in the quantum dot under a magnetic field. We propose the conception of magneto-bipolaron qubit in the quantum dot made of I–VII semiconductors, complement and perfect the phonon effect of solid state quantum information.

2. Theoretical model and method

We consider a two-electron system which is restrained in a two-dimension (x–y plane) parabolic quantum dot and inter-

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acts with the longitudinal optical (LO) phonon. The external magnetic field $\boldsymbol{B}$ is along the z direction. The vector potential is $\boldsymbol{A} = B(-y,x,0)/2$. We set the center of the quantum dot as origin point O to establish the plane polar coordinates, see Fig. 1. The system's Frölich Hamiltonian[20,21] can be written as

$$\begin{aligned} H &= \sum_{j=1}^{2}\left[\frac{1}{2m_{\rm b}}(\boldsymbol{p}_j + e\boldsymbol{A}_j)^2 + \frac{1}{2}m_{\rm b}\omega_0^2\rho_j^2 + \sum_{k_j}\hbar\omega_{\rm LO}a_{k_j}^{+}a_{k_j}\right. \\ &\quad \left. + \sum_{k_j}(v_{k_j}a_{k_j}\,{\rm e}^{{\rm i}\boldsymbol{k}_j\cdot\boldsymbol{\rho}_j} + v_{k_j}^{*}a_{k_j}^{+}\,{\rm e}^{-{\rm i}\boldsymbol{k}_j\cdot\boldsymbol{\rho}_j})\right] + \frac{e^2}{\varepsilon_\infty|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}. \end{aligned} \tag{1}$$

In the above expression, the four terms in the summation represent the single-electron kinetic energy, the confinement potential of the quantum dot, the energy of the local LO phonon field, and the electron–LO phonon interaction, respectively. The last term represents the Coulomb interaction energy between the two electrons. Here, $\boldsymbol{p}_j$ and $\boldsymbol{\rho}_j$ $(j=1,2)$ are respectively the momentum and position vectors of the two electrons, ω_0 is the confinement strength, and $a_{k_j}^{+}$ (a_{k_j}) denotes the creation (annihilation) operator of the LO phonon with wave vector k_j and frequency $\omega_{\rm LO}$. The interaction coefficient is

$$v_{k_j} = \frac{\hbar\omega_{\rm LO}}{k_j}\left[\frac{4\pi\alpha}{V}\left(\frac{\hbar}{2m_{\rm b}\omega_{\rm LO}}\right)^{1/2}\right]^{1/2}, \tag{2}$$

where V is the volume of the crystal, and α is the dimensionless electron–LO phonon coupling strength

$$\alpha = \frac{e^2}{2\hbar r_{\rm p}\omega_{\rm LO}}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right),\quad r_{\rm p} = \left(\frac{\hbar}{2m_{\rm b}\omega_{\rm LO}}\right)^{1/2}, \tag{3}$$

with ε_∞ (ε_0) being the high-frequency (static) dielectric constant of the medium and $r_{\rm p}$ being the radius of the polaron.

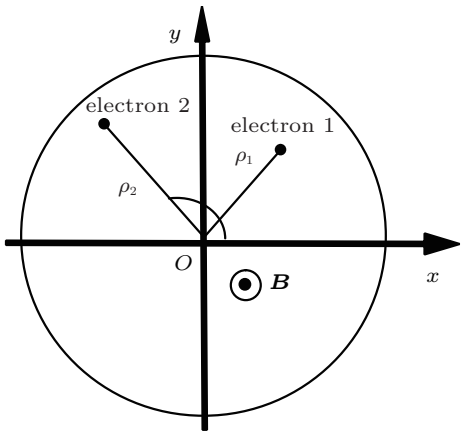


Fig. 1. Schematic diagram of quantum dot.

To obtain the system energy, the extremum problem about the expectation value of the variational function $U^{-1}HU$ in the state $|\Psi\rangle$ is discussed here. According to the variational principle,

$$\delta\bar{H} = \delta\langle\Psi|U^{-1}HU|\Psi\rangle = 0, \tag{4}$$

where

$$U = \exp\left[\sum_{k_j}\left(f_{k_j}a_{k_j}^{+} - f_{k_j}^{*}a_{k_j}\right)\right] \tag{5}$$

is the Lee–Low–Pines unitary transformation[22] with variational parameters f_{k_j} and $f_{k_j}^{*}$. For the ground and the first-excited states of the system, it is assumed that the Gaussian function is approximately tenable. According to the variational method of Pekar type,[23,24] the trial wave-functions of the system in the ground state and the first-excited state can be respectively chosen as

$$\begin{aligned} &|\Psi_{00}\rangle = \psi_0(\boldsymbol{\rho}_1)\psi_0(\boldsymbol{\rho}_2)|0_{\rm ph}\rangle, \\ &\psi_0(\boldsymbol{\rho}_j) = \frac{\lambda_0}{\sqrt{\pi}}\exp\left(-\frac{\lambda_0^2\rho_j^2}{2}\right),\quad (j=1,2); \end{aligned} \tag{6}$$

$$\begin{aligned} &|\Psi_{01}\rangle = \psi_0(\boldsymbol{\rho}_1)\psi_1(\boldsymbol{\rho}_2)|0_{\rm ph}\rangle, \\ &\psi_1(\boldsymbol{\rho}_j) = \frac{\lambda_1^2}{\sqrt{\pi}}\rho_j\exp\left(-\frac{\lambda_1^2\rho_j^2}{2}\right)\exp(\pm{\rm i}\varphi_j),\quad (j=1,2); \end{aligned} \tag{7}$$

where λ_0 and λ_1 are the variational parameters, $\psi_0(\boldsymbol{\rho}_j)$ and $\psi_1(\boldsymbol{\rho}_j)$ are the ground state and the first-excited state trial wave-functions of the electron, and $|0_{\rm ph}\rangle$ is the unperturbed zero phonon state. By substituting Eqs. (1)–(3) and (5)–(7) into Eq. (4), every variational parameter can be obtained. Then the energies of the ground state and the first excited state are derived by tedious calculations to be

$$\begin{aligned} E_0(\lambda_0) &= \langle\Psi_{00}|H|\Psi_{00}\rangle \\ &= \left(2r_{\rm p}^2\lambda_0^2 + \frac{\omega_0^2}{2r_{\rm p}^2\lambda_0^2\omega_{\rm LO}^2} + \frac{\omega_{\rm c}^2}{8r_{\rm p}^2\lambda_0^2\omega_{\rm LO}^2} - \sqrt{2\pi}\alpha r_{\rm p}\lambda_0\right)\hbar\omega_{\rm LO} \\ &\quad + E_{\rm c}^{(0)}, \end{aligned} \tag{8}$$

$$\begin{aligned} E_1(\lambda_0,\lambda_1) &= \langle\Psi_1|H|\Psi_1\rangle \\ &= \left(r_{\rm p}^2\lambda_0^2 + \frac{\omega_0^2}{4r_{\rm p}^2\lambda_0^2\omega_{\rm LO}^2} - \sqrt{\frac{\pi}{2}}\alpha r_{\rm p}\lambda_0 + 2r_{\rm p}^2\lambda_1^2\right. \\ &\quad \left. + \frac{\omega_0^2}{2r_{\rm p}^2\lambda_1^2\omega_{\rm LO}^2} + \frac{\omega_{\rm c}^2}{8r_{\rm p}^2\lambda_1^2\omega_{\rm LO}^2} - \frac{11}{32}\sqrt{2\pi}\alpha r_{\rm p}\lambda_1\right)\hbar\omega_{\rm LO} + E_{\rm c}^{(1)}, \end{aligned} \tag{9}$$

$$\begin{aligned} E_{\rm c}^{(0)} &= \frac{2\lambda_0^4 r_{\rm p}^4\alpha\hbar\omega_{\rm LO}}{\pi^2(1-\eta)}\int_0^\infty{\rm d}x_1\int_0^\infty{\rm d}x_2\int_0^{2\pi}{\rm d}\varphi_1\int_0^{2\pi}{\rm d}\varphi_2\,x_1x_2 \\ &\quad \times\frac{\exp\left(-\frac{x_1^2+x_2^2}{2}r_{\rm p}^2\lambda_0^2\right)}{\sqrt{x_1^2+x_2^2-2x_1x_2\cos(\varphi_1-\varphi_2)}}, \end{aligned} \tag{10}$$

$$\begin{aligned} E_{\rm c}^{(1)} &= \frac{2\lambda_0^2\lambda_1^4 r_{\rm p}^6\alpha\hbar\omega_{\rm LO}}{\pi^2(1-\eta)}\int_0^\infty{\rm d}x_1\int_0^\infty{\rm d}x_2\int_0^{2\pi}{\rm d}\varphi_1\int_0^{2\pi}{\rm d}\varphi_2\,x_1x_2^3 \end{aligned}$$

$$\times \frac{\exp\left(-\frac{\lambda_0^2 x_1^2+\lambda_1^2 x_2^2}{2} r_{\rm p}^2\right)}{\sqrt{x_1^2+x_2^2-2x_1x_2\cos(\varphi_1-\varphi_2)}}, \tag{11}$$

where $\eta=\varepsilon_\infty/\varepsilon_0$ is the dielectric constant ratio of the medium, and $\omega_{\rm c}=eB/m_{\rm b}c$ is the resonant frequency of the magnetic field. So, a two-level system as a single qubit is built up. The superposition state of electron can be expressed as

$$\Psi(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,t) = \frac{1}{\sqrt{2}}\left[|\Psi_{00}\rangle\exp\left(-{\rm i}\frac{E_0}{\hbar}t\right)+|\Psi_{01}\rangle\exp\left(-{\rm i}\frac{E_1}{\hbar}t\right)\right]. \tag{12}$$

The probability density of the two electrons in the qubit is in the following form:

$$Q(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,t)=|\Psi(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,t)|^2. \tag{13}$$

The oscillation period of the probability density is

$$T_0=\frac{2\pi\hbar}{E_1-E_0}. \tag{14}$$

3. Results and discussion

To show the variations of E_0, E_1, Q, and T_0 with $\omega_{\rm c}$, ω_0, η, and α clearly and intuitively, the results of numerical calculations are shown in Figs. 2–7, taking $\hbar\omega_{\rm LO}$ as the unit of energy, $\omega_{\rm LO}$ as the unit of ω_0 and $\omega_{\rm c}$, and $r_{\rm p}$ as the length unit.

Figure 2 shows the variations of the ground state energy E_0 and the first-excited state energy E_1 of magneto-bipolaron with (a) the confinement strength ω_0 at different electron–phonon coupling strength α and (b) the dielectric constant ratio η at different resonant frequency of the magnetic field $\omega_{\rm c}$. From Figs. 2(a) and 2(b), it can be seen that the ground state energy of magneto-bipolaron $E_0<0$, and the absolute value of E_0 is very large. This indicates that the ground state of magneto-bipolaron is a steady bound state and needs huge energy to excite it, so the first-excited state of magneto-bipolaron should be structured by one electron staying in the ground state and the other electron being excited to the first-excited state. This is why we use Eq. (6) as the ground state trial wave-function of magneto-bipolaron and Eq. (7) as the first-excited state trial wave-function. It can be seen from Fig. 2(a) that the absolute value of the ground state energy $|E_0|$ decreases with increasing ω_0, while the first-excited state energy E_1 increases with increasing ω_0. $|E_0|$ and E_1 increase with increasing α when ω_0 is fixed. It can be seen from Fig. 2(b) that $|E_0|$ and E_1 increase with increasing η. When η is fixed, $|E_0|$ decreases with increasing $\omega_{\rm c}$, but E_1 increases with increasing $\omega_{\rm c}$.

Figure 3 shows the variations of the oscillation period T_0 with (a) the confinement strength ω_0 at different electron–phonon coupling strength α and (b) the dielectric constant ratio η at different resonant frequency of the magnetic field $\omega_{\rm c}$. It can be seen from Fig. 3(a) that T_0 decreases with increasing ω_0 and α. This is because the energy difference $\Delta E=E_1-E_0$ increases with increasing ω_0 and α, which can be seen from Fig. 2(a). It can be seen from Fig. 3(b) that T_0 decreases with increasing η and $\omega_{\rm c}$. This is because the energy difference $\Delta E=E_1-E_0$ increases with increasing η and $\omega_{\rm c}$, which can be seen from Fig. 2(b). Here we can see that the magneto-bipolaron qubit coherence decreases with increasing confinement strength of the quantum dot, electron–phonon coupling strength, dielectric constant ratio, and external magnetic field. This is in agreement with the discussion in Refs. [15]– [18].

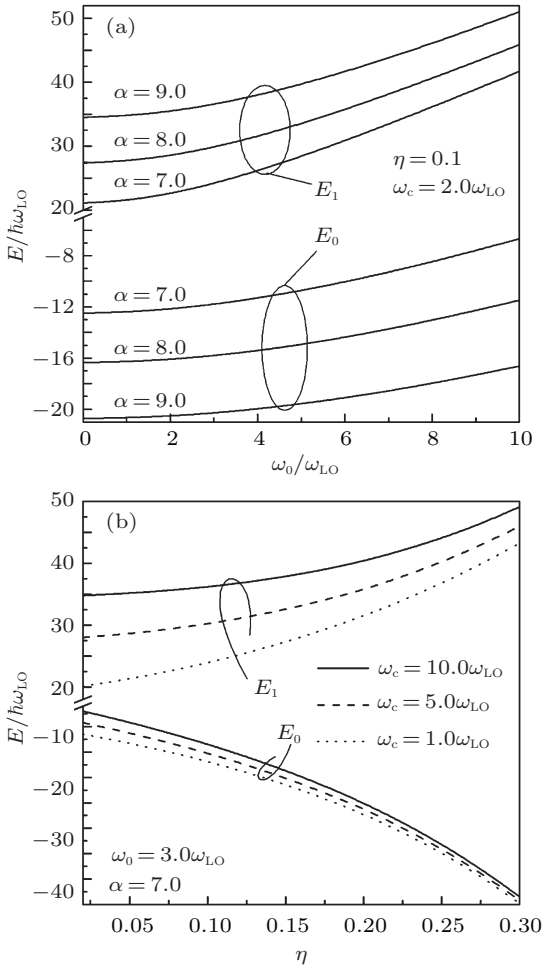


Fig. 2. Variations of the ground state energy E_0 and the first-excited state energy E_1 of magneto-bipolaron with (a) the confinement strength ω_0 at different electron–phonon coupling strength α and (b) the dielectric constant ratio η at different resonant frequency of the magnetic field $\omega_{\rm c}$.

Figure 4 shows the variations of the probability density Q with (a) the confinement strength ω_0 and (b) the dielectric constant ratio η. It can be seen from Fig. 4(a) that Q first increases to a maximum and then quickly decreases to a minimum and finally increases again in a very short time. From Fig. 4(b), it is not difficult to see that Q increases oscillatory with increasing η.

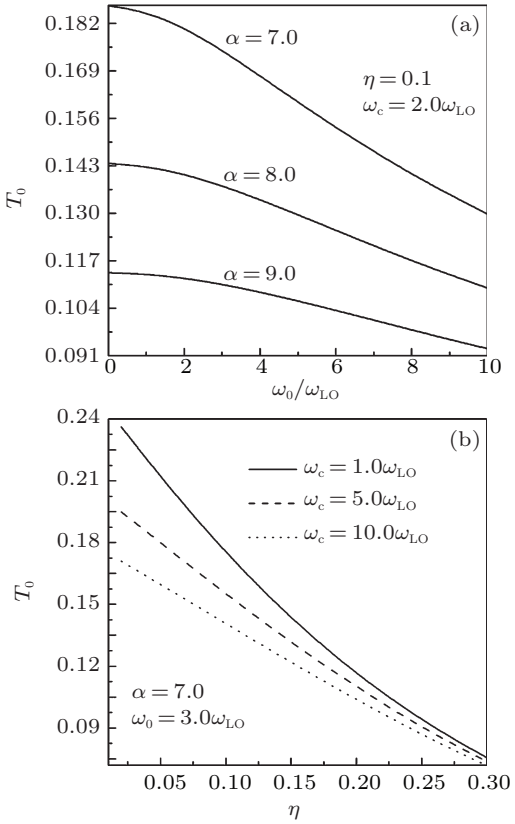


Fig. 3. Variations of the oscillation period T_0 with (a) the confinement strength ω_0 at different electron–phonon coupling strength α and (b) the dielectric constant ratio η at different resonant frequency of the magnetic field ω_c.

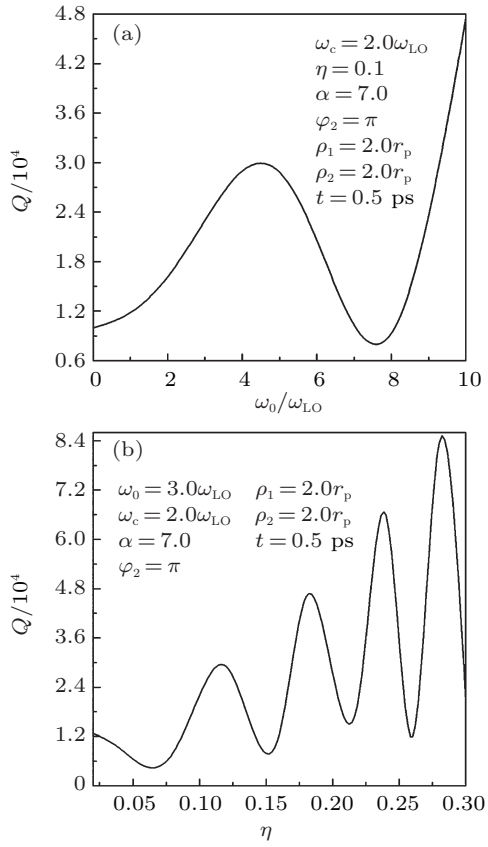


Fig. 4. Variations of the probability density Q with (a) the confinement strength ω_0 and (b) the dielectric constant ratio η.

Figure 5 shows the variations of the probability density Q with (a) polar angle φ_2 and (b) time t. From Fig. 5, it can be seen that Q oscillates periodically with increasing φ_2 or t.

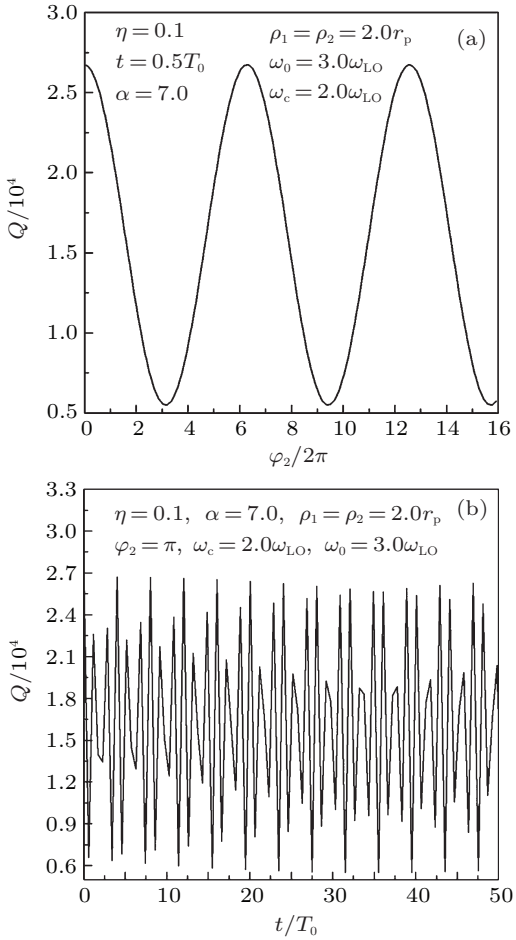


Fig. 5. Variations of the probability density Q with (a) polar angle φ_2 and (b) time t.

From Figs. 4 and 5, we can find that the probability density Q of the two electrons in the qubit oscillates periodically with increasing time t, angular coordinate φ_2, and dielectric constant ratio of the medium η. Physically, it is a representation of volatility of bipolaron superposition state. To be specific, the phase change of the probability wave of bipolaron depends on time t.

Figure 6 shows the variations of the probability density Q with coordinate ρ_1 at (a) different electron–phonon coupling strength α and (b) different resonant frequency of the magnetic field ω_c. From Fig. 6(a), it can be seen that Q quickly decreases with increasing ρ_1 and α has certain influence on the change of Q with ρ_1. From Fig. 6(b), it is not difficult to see that ω_c also has certain influence on the change of Q with ρ_1. From Fig. 6, we find that the probability of electron 1 appearing near the center of the quantum dot ($\rho_1 < 6.0r_p$) is larger, and the probability of appearing away from the center of the quantum dot is smaller.

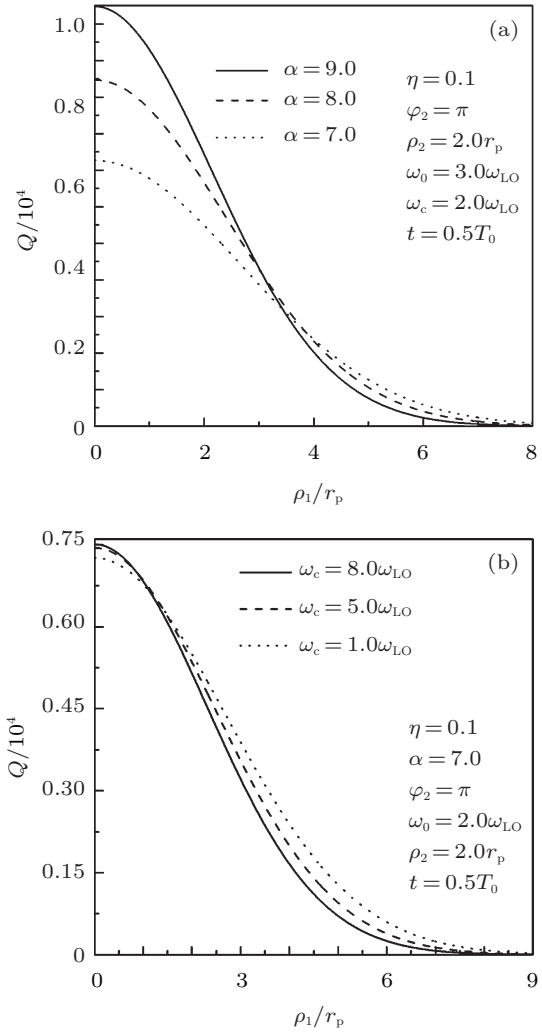


Fig. 6. Variations of the probability density Q with coordinate ρ_1 at (a) different electron–phonon coupling strength α and (b) different resonant frequency of the magnetic field ω_c.

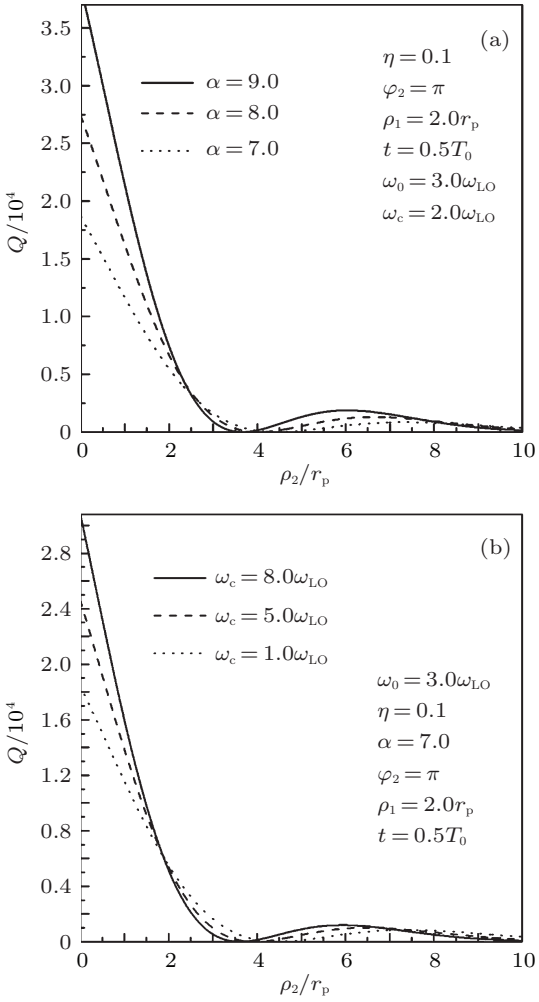


Fig. 7. Variations of the probability density Q with coordinate ρ_2 at (a) different electron–phonon coupling strength α and (b) different resonant frequency of the magnetic field ω_c.

Figure 7 shows the variations of the probability density Q with coordinate ρ_2 at (a) different electron–phonon coupling strength α and (b) different resonant frequency of the magnetic field ω_c. From Fig. 7(a), it can be seen that Q first quickly decreases to a minimum and then slowly increases to a maximum and finally decreases slowly to zero. In the meantime, α has certain influence on the change of Q with ρ_2. From Fig. 7(b), it can be seen that the variations of Q with ρ_2 at different ω_c is very similar to those at different α in Fig. 7(a). From Fig. 7, we find that the probability of electron 2 appearing near the center of the quantum dot ($\rho_2 < 3.0r_p$) is larger, and the range of electron 2 is smaller than that of electron 1, and the probability of appearing away from the center of the quantum dot is smaller. Here we can see that the probability of electron appearing near the center of the quantum dot is larger. This is because the harmonic confinement potential of the quantum dot is smaller in the central area and the system energy is lower when the electrons are at the central area.

4. Conclusion

Based on the variational method of Pekar type, we study the energies and the wave-functions of the ground and the first-excited states of magneto-bipolaron, which is strongly coupled to the LO phonon in a parabolic potential quantum dot under an applied magnetic field, thus built up a quantum dot magneto-bipolaron qubit. The following results are obtained. (i) The oscillation period of the probability density of the two electrons in the qubit decreases with increasing electron–phonon coupling strength α, resonant frequency of the magnetic field ω_c, confinement strength of the quantum dot ω_0, and dielectric constant ratio of the medium η. (ii) The probability density of the two electrons in the qubit oscillates periodically with increasing time t, angular coordinate φ_2, and dielectric constant ratio of the medium η. (iii) The probability of electron appearing near the center of the quantum dot is larger, and the probability of electron appearing away from the center of the quantum dot is much smaller.

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