Characteristics of strong-coupling bipolaron qubit in two-dimensional quantum dot in electric field*

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Based on Lee-Low-Pines (LLP) unitary transformation, this article adopts the variational method of the Pekar type and gets the energy and wave functions of the ground state and the first excited state of strong-coupling bipolaron in two-dimensional quantum dot in electric field, thus constructs a bipolaron qubit. The numerical results represent that the time oscillation period T_0 of probability density of the two electrons in qubit decreases with the increasing electric field intensity F and dielectric constant ratio of the medium η; the probability density Q of the two electrons in qubit oscillates periodically with the increasing time t; the probability of electron appearing near the center of the quantum dot is larger, while that appearing away from the center of the quantum dot is much smaller.
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In recent years, people put forward various solutions to get qubit, for example, ion traps[1], nuclear spins and electrons[2,3], quantum dot[4], etc. Among them, the quantum-dot quantum computer can be used as the basic unit of the quantum optical technology because its energy level structures are adjustable and it can realize the all-optical operation and integration of the qubit. Therefore, many scholars have done various researches on such quantum dot qubit and got a series of important results. Jordan et al[5] studied the coherent rotations of a single-spin qubit at fixed Zeeman energy. Furuta et al[6] discussed the single-qubit gate and measurement of the surface acoustic wave quantum computer. Li et al[7,8] proposed to use external electric field to increase the decoherence time of quantum dot qubit. And in recent years, people studied the influence of the interaction of electron and phonon in quantum dot on the qubit. Xiao[9] studied the effect of electric field on an asymmetric quantum dot qubit. Sun et al[10] studied the effects of magnetic field on the decoherence time of parabolic quantum dot qubit. So far as we know, there is no report about the study of bipolaron qubit in quantum dot. In fact, most artificial low-dimensional structures are prepared by ionic crystal or polar semiconductor and they strengthen the electron-phonon interaction in quantum dot structure by the decrease of dimension, which enables two identical electrons to form bipolaron bound state[11,12] through the phonon field interaction.

This article adopts the variational method of the Pekar type based on the Lee-Low-Pines (LLP) unitary transformation to study the properties of the qubit structured by strong-coupling bipolaron ground state and the first excited state in two-dimensional quantum dot in electric field.

Considering that the two-electron system is restrained in a two-dimension ($x-y$ plane) parabolic quantum dot and interacts with longitudinal optical (LO) phonon, we set the external electronic field along the x axis and set the center of quantum dot as origin point O to establish the plane polar coordinates, as shown in Fig.1. The system's Frölich Hamiltonian[12] can be written as:

$$H=\sum_{j=1}^{2}\left[\frac{\boldsymbol{p}_j^2}{2m_{\mathrm{b}}}+\frac{1}{2}m_{\mathrm{b}}\omega_0^2\boldsymbol{\rho}_j^2+\sum_{\boldsymbol{k}_j}\hbar\omega_{\mathrm{LO}}a_{\boldsymbol{k}_j}^{+}a_{\boldsymbol{k}_j}+\right.$$
$$\left.\sum_{\boldsymbol{k}_j}\left(v_{\boldsymbol{k}_j}a_{\boldsymbol{k}_j}\mathrm{e}^{\mathrm{i}\boldsymbol{k}_j\cdot\boldsymbol{\rho}_j}+v_{\boldsymbol{k}_j}^{*}a_{\boldsymbol{k}_j}^{+}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_j\cdot\boldsymbol{\rho}_j}\right)-\mathrm{e}Fx_j\right]+\frac{\mathrm{e}^2}{\varepsilon_\infty|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|}\quad .\ (1)$$

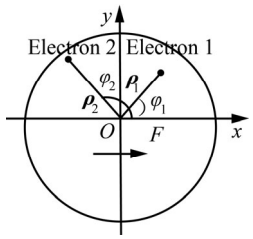

Fig1. Schematic diagram of quantum dot

In the above expression, the five items in the right summation symbol represent the single-electron kinetic energy, confinement potential of quantum dots, energy of

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local LO phonon field, electron-LO phonon interaction term, and the additional energy caused by electric field; the last item represents the Coulomb interaction energy of two electrons. $\boldsymbol{p}_j$ and $\boldsymbol{\rho}_j$ ($j=1,\ 2$) respectively are the momentum and coordinates of the two electrons in $x-y$ plane. ω_0 is the confinement potential strength of the electron from quantum dot. $a_{\boldsymbol{k}_j}^{+}$ and $a_{\boldsymbol{k}_j}$ are the operators of creation and annihilation of the LO phonon with the wave vector of $\boldsymbol{k}_j$ and frequency of ω_{LO}. The interaction coefficient is

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

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

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

where ε_∞ (ε_0) is the high-frequency (static) dielectric constant of the medium and r_{p} is the radius of the polaron.

In order to get the system energy and discuss the extremum problem of the expected value $\bar{H}$ of the variational function $U^{-1}HU$ in the state $|\psi\rangle$, we adopt the variational principle of

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

where

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

is the Lee-Low-Pines (LLP) unitary transformation[13], in which $f_{\boldsymbol{k}_j}$ and $f_{\boldsymbol{k}_j}^{*}$ are the variational parameters. We assume that the Gaussian function is approximately valid for the ground state and first excited state of the system, then according to the variational method of Pekar type[14], the ground state trial wave function $|\Psi_{00}\rangle$ and the first excited state trial wave function $|\Psi_{01}\rangle$ of the system can respectively be chosen as

$$|\Psi_{00}\rangle=\Psi_0(\boldsymbol{\rho}_1)\Psi_0(\boldsymbol{\rho}_2)|0_{\mathrm{ph}}\rangle,$$

$$\Psi_0(\boldsymbol{\rho}_j)=\frac{\lambda_0}{\sqrt{\pi}}\exp\left(-\frac{\lambda_0^2\boldsymbol{\rho}_j^2}{2}\right),\ (j=1,\ 2), \tag{6}$$

$$|\Psi_{01}\rangle=\Psi_0(\boldsymbol{\rho}_1)\Psi_1(\boldsymbol{\rho}_2)|0_{\mathrm{ph}}\rangle,$$

$$\Psi_1(\boldsymbol{\rho}_j)=\frac{\lambda_1^2}{\sqrt{\pi}}\boldsymbol{\rho}_j\exp\left(-\frac{\lambda_1^2\boldsymbol{\rho}_j^2}{2}\right)\exp(\pm\mathrm{i}\phi_j),$$

$$(j=1,\ 2), \tag{7}$$

where λ_0 and λ_1 are the variational parameters. $\psi_0(\boldsymbol{\rho}_j)$ and $\psi_1(\boldsymbol{\rho}_j)$ represent the ground state trial wave function and the first excited state trial wave function of a single electron. $|0_{\mathrm{ph}}\rangle$ is the vacuum state of phonon. Substituting Eqs.(1)–(3) and (5)–(7) into Eq.(4), we can get the variational parameters of $f_{\boldsymbol{k}}$, $f_{\boldsymbol{k}}^{*}$, λ_1 and λ_2. And through expatiatory calculation, we can know that the ground state energy and first excited state energy of the bipolaron system are

$$E_0(\lambda_0)=\langle\Psi_{00}|H|\Psi_{00}\rangle=\left(2r_{\mathrm{p}}^2\lambda_0^2+\frac{\omega_0^2}{2r_{\mathrm{p}}^2\lambda_0^2\omega_{\mathrm{LO}}^2}-\right.$$

$$\left.\sqrt{2\pi}\alpha r_{\mathrm{p}}\lambda_0-\frac{F}{\sqrt{\pi}r_{\mathrm{p}}\lambda_0R^*}\right)\hbar\omega_{\mathrm{LO}}+E_{\mathrm{c}}^{(0)}, \tag{8}$$

$$E_1(\lambda_0,\lambda_1)=\langle\Psi_1|H|\Psi_1\rangle=\left(r_{\mathrm{p}}^2\lambda_0^2+\frac{\omega_0^2}{4r_{\mathrm{p}}^2\lambda_0^2\omega_{\mathrm{LO}}^2}-\right.$$

$$\sqrt{\frac{\pi}{2}}\alpha r_{\mathrm{p}}\lambda_0-\frac{F}{4r_{\mathrm{p}}\lambda_1R^*}+2r_{\mathrm{p}}^2\lambda_1^2+$$

$$\left.\frac{\omega_0^2}{2r_{\mathrm{p}}^2\lambda_1^2\omega_{\mathrm{LO}}^2}-\frac{11}{32}\sqrt{2\pi}\alpha r_{\mathrm{p}}\lambda_1\right)\hbar\omega_{\mathrm{LO}}+E_{\mathrm{c}}^{(1)}, \tag{9}$$

$$E_{\mathrm{c}}^{(0)}=\frac{2\lambda_0^4r_{\mathrm{p}}^4\alpha\hbar\omega_{\mathrm{LO}}}{\pi^2(1-\eta)}\int_0^\infty\mathrm{d}x_1\int_0^\infty\mathrm{d}x_2\int_0^{2\pi}\mathrm{d}\varphi_1\int_0^{2\pi}\mathrm{d}\varphi_2\times$$

$$\frac{x_1x_2\exp\left(-\frac{x_1^2+x_2^2}{2}r_{\mathrm{p}}^2\lambda_0^2\right)}{\sqrt{x_1^2+x_2^2-2x_1x_2\cos(\varphi_1-\varphi_2)}}, \tag{10}$$

$$E_{\mathrm{c}}^{(1)}=\frac{2\lambda_0^2\lambda_1^4r_{\mathrm{p}}^6\alpha\hbar\omega_{\mathrm{LO}}}{\pi^2(1-\eta)}\int_0^\infty\mathrm{d}x_1\int_0^\infty\mathrm{d}x_2\int_0^{2\pi}\mathrm{d}\varphi_1\int_0^{2\pi}\mathrm{d}\varphi_2\times$$

$$\frac{x_1x_2^3\exp\left(-\frac{\lambda_0^2x_1^2+\lambda_1^2x_2^2}{2}r_{\mathrm{p}}^2\right)}{\sqrt{x_1^2+x_2^2-2x_1x_2\cos(\varphi_1-\varphi_2)}}, \tag{11}$$

in which $\eta=\varepsilon_\infty/\varepsilon_0$ is dielectric constant ratio of the medium, $R^*=\hbar\omega_{\mathrm{LO}}/\mathrm{e}r_{\mathrm{p}}$. Thus, we can establish a two-level system. When the electron is in superposition state

$$\Psi(\boldsymbol{\rho}_1,\boldsymbol{\rho}_2,t)=$$

$$\frac{1}{\sqrt{2}}\left[|\Psi_{00}\rangle\exp\left(-\mathrm{i}\frac{E_0}{\hbar}t\right)+|\Psi_{01}\rangle\exp\left(-\mathrm{i}\frac{E_1}{\hbar}t\right)\right], \tag{12}$$

it establishes a quantum dot bipolaron qubit. The probability density of the two electrons in qubit is

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

whose time oscillation period T_0 is

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

The results of numerical calculation are given in Figs.2 to 5, taking $\hbar\omega_{LO}$ as the unit of energy, $R^* = \hbar\omega_{LO}/er_p$ as the unit of electric field intensity F, ω_{LO} as the unit of ω_0 and r_p as the length unit.

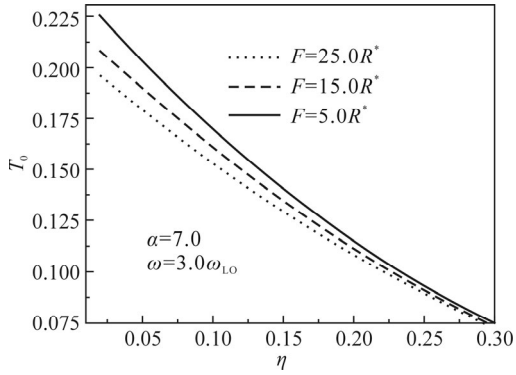

Fig.2 Variation of oscillation period T_0 with the dielectric constant ratio η at different electronic field intensities F

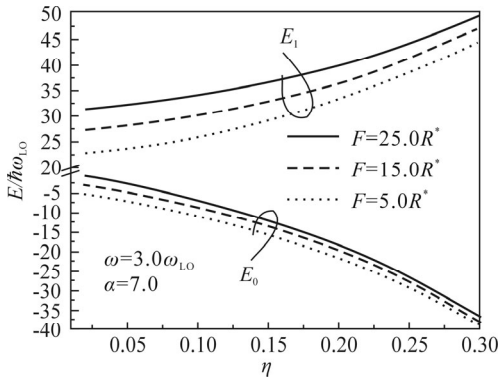

Fig.3 Variations of the ground state energy E_0 and the first excited state energy E_1 of bipolaron with the dielectric constant ratio η at different electronic field intensities F

In Fig.2, we can get that T_0 decreases with the increasing η. In Fig.3, E_1 increases with increasing η, but E_0 decreases, so the energy level difference $\Delta E=E_1-E_0$ increases with increasing η, which causes T_0 to decrease with increasing η. When η is given, T_0 decreases with increasing F. From Fig.3, we can get that E_1 increases quickly with increasing F, but the ground state energy is negative, whose absolute value $|E_0|$ ecreases with increasing F, so the energy level difference $\Delta E=E_1-E_0$ increases with increasing F, which causes T_0 to decrease with increasing F. Thus we can get the conclusion: the external electric field and the dielectric constant ratio both can decrease the coherence of bipolaron qubit, which agrees with the result of monopolaron quantum dot qubit from Refs.[9,10].

Fig.4 describes the variation of the probability density Q with time t From Fig.4, we can get that Q makes the amplitude modulation oscillated with period T_0.

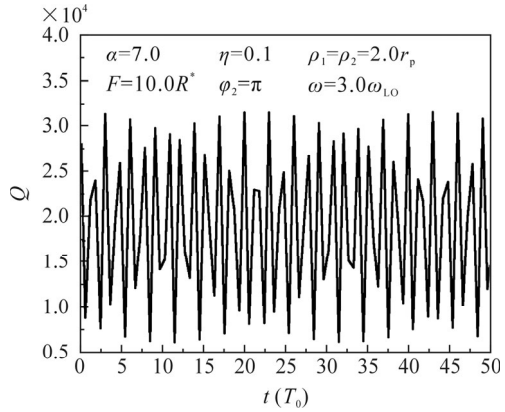

Fig.4 Variation of the probability density Q with time t

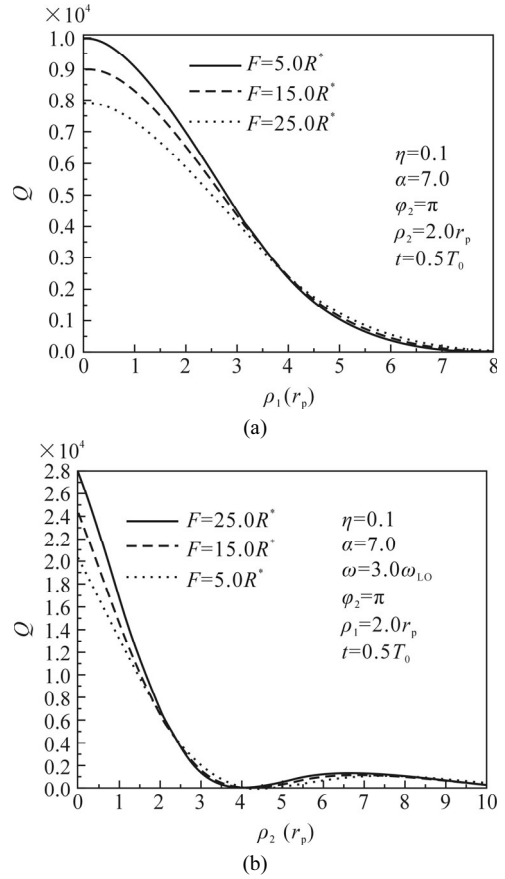

Fig.5 Variations of the probability density Q with (a) coordinate ρ_1 and (b) coordinate ρ_2 at different electronic field intensities F

From Fig.5(a), it's easy to see that F has a certain influence on the changes of Q with ρ_1, which means that $Q-\rho_1$ curves corresponding to different F values move down with increasing F. We can get that the probability of electron 1 appearing near the center of the quantum dot ($\rho_1 < 6.0r_p$) is larger, while the probability of it appearing away from the center of the quantum dot is smaller. In Fig.5(b), we can get the following conclusion: the probability of electron 2 appearing near the center of the quantum dot ($\rho_2 < 3.0r_p$) is larger, but the appearing range of electron 2 is smaller than that of electron 1.

In conclusion, this paper takes the external electric field into consideration and discusses two electron systems which are bound in two-dimension parabolic potential quantum dot and made strong-coupling with LO phonon (the electron-phonon coupling strength is $\alpha > 6.0$). We adopt the variational method of the Pekar type based on LLP unitary transformation and get the energy and wave functions of the ground state and the first excited state of strong-coupling bipolaron, thus construct a quantum dot bipolaron qubit. The numerical results represent that the time oscillation period T_0 of probability density of the two electrons in qubit decreases with the increasing electric field intensity F and the dielectric constant ratio of the medium η; the probability density Q of the two electrons in qubit oscillates periodically with the increasing time t; the probability of electron appearing near the center of the quantum dot is larger, while that appearing away from the center of the quantum dot is much smaller.

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