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Magnetic field effect on state energies and transition frequency of a strong-coupling polaron in an anisotropic quantum dot

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Abstract. By employing a variational method of the Pekar-type, which has different variational parameters in the x–y plane and the z-direction, we study the ground and the first excited state energies and transition frequency between the ground and the first excited states of a strong-coupling polaron in an anisotropic quantum dot (AQD) under an applied magnetic field along the z-direction. The effects of the magnetic field and the electron–phonon coupling strength are taken into account. It is found that the ground and the first excited state energies and the transition frequency are increasing functions of the external applied magnetic field. The ground state and the first excited state energies are decreasing functions, whereas transition frequency is an increasing function of the electron–phonon coupling strength. We find two ways of tuning the state energies and the transition frequency: by adjusting (1) the magnetic field and (2) the electron–phonon coupling strength.

Keywords. Anisotropic quantum dots; polaron; variational method of the Pekar-type; magnetic field.

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1. Introduction

In the past decades, both experimental [1–6] and theoretical [7–9] physicists showed growing interest in studying the eigenenergies and the relevant eigenfunctions of an electron's ground and first excited states in low-dimensional nanostructures. This two-level system may be used as a two-level quantum qubit. QDs have attracted lots of research interest due to their wide quantum functional device applications and many new physical characteristics. In the framework of effective-mass envelope function theory, Li and Xia [10] theoretically investigated the electronic structures of N quantum dot molecule, and calculated the electron and hole energy levels. The interplay between confinement

effects due to applied electric and magnetic fields, quantum-size confinements, and the electron–phonon coupling on the impurity binding energy were analysed by Vartanian *et al* [11]. Analytical expression for polaron energy had been obtained as a function of the QD sizes, intensities of the applied fields, and the position of the impurity in the QD. Kaczmarkiewicz and Machnikowski [12] theoretically studied the resonant features in the spectrum of an electron confined in a self-assembled QD and interacting with LO phonons. They had focussed on the second-order resonance induced by the indirect interaction between the first-excited electronic shell (p shell) and the electronic ground state with two LO phonons, and calculated this second-order resonant polaron spectrum as a function of the dot size and external magnetic field. By using the invariant theory, Yu and Jiao [13] investigated the geometric phase of QDs in the time-dependent isotropic magnetic field. Considering the Gaussian impurity centers, Datta and Ghosh [14] explored the excitation profile of a repulsive impurity-doped QD under randomly fluctuating magnetic field. Their investigation revealed the roles subtly played by the dopant coordinate, dopant strength, and the region of influence of the dopant to modulate the excitation pattern. Utilizing the Aldrich–Bajaj effective potential, Kumar *et al* [15] investigated the effect of LO phonon field on the ground state and low-lying excited state energies of a hydrogenic impurity in a $Zn_{1-x}Cd_xSe/ZnSe$ strained QD for various Cd concentrations. Khordad [16] had considered an exciton confined in a spherical QD with the modified Gaussian potential and studied the electronic and optical properties of the system using the numerical diagonalization of the Hamiltonian matrix. Based on the linear combination operator method, we have calculated the vibrational frequency, the ground state energy, and the ground state binding energy of the strong-coupling impurity magnetopolaron in an AQD [17].

Since Landau and Pekar first investigated the properties of the strong coupling polaron by the variational method of the Pekar-type [18,19], many researchers had studied the polaron problems by this method [20–23]. However, the properties of the magnetopolaron in an AQD have not been studied so far by employing variational method.

In this paper, by employing the variational method of the Pekar-type, which has different variational parameters in the x–y plane and the z-direction, we study the effects of magnetic field on the ground and the first excited state energies and the transition frequency of a strong-coupling polaron in an AQD.

2. Theory model and calculations

The electron under consideration is moving in a polar crystal AQD with three-dimensional anisotropic harmonic potential, and interacting with bulk LO phonons, under the influence of a magnetic field along the z-direction with vector potential of $\mathbf{A} = B\,(-y/2, x/2, 0)$. The Hamiltonian of the electron–phonon interaction system can be written as

$$H = \frac{1}{2m}\left(p_x - \frac{\bar{\beta}^2}{4}y\right)^2 + \frac{1}{2m}\left(p_y + \frac{\bar{\beta}^2}{4}x\right)^2 + \frac{p_z^2}{2m} + \sum_{\mathbf{q}} \hbar\omega_{\mathrm{LO}} a_{\mathbf{q}}^{+} a_{\mathbf{q}} + \frac{1}{2}m\omega_1^2\rho^2 + \frac{1}{2}m\omega_2^2 z^2 + \sum_{\mathbf{q}}\left[V_q a_{\mathbf{q}} \exp(i\mathbf{q}\cdot\mathbf{r}) + \mathrm{h.c.}\right], \quad (1)$$

where $\bar{\beta}^2 = (2e/c)B$ and m is the band mass, ω_1 and ω_2 are the magnitude of the transverse and longitudinal confinement strengths of the potentials in the x–y plane and the z-direction, respectively. $a_{\mathbf{q}}^{+}(a_{\mathbf{q}})$ denotes the creation(annihilation) operator of the bulk LO phonon with wave vector $\mathbf{q}$, $\mathbf{P} = (P_x, P_y, P_z)$ and $\mathbf{r} = (\boldsymbol{\rho}, z)$ are the momentum and position vector of the electron, $\boldsymbol{\rho} = (x, y)$ is the position vector of the electron in the x–y plane. V_q and α in eq. (1) are

$$V_q = i\left(\frac{\hbar\omega_{\mathrm{LO}}}{q}\right)\left(\frac{\hbar}{2m\omega_{\mathrm{LO}}}\right)^{1/4}\left(\frac{4\pi\alpha}{V}\right)^{1/2},$$

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{\mathrm{LO}}}\right)\left(\frac{2m\omega_{\mathrm{LO}}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \tag{2}$$

Following the Pekar variational method, the trial wave function of the strong-coupling polaron can be separated into two parts, which individually describes the electron and the phonon. The trial wave function can be written as [24]

$$|\psi\rangle = |\varphi\rangle U|0_{\mathrm{ph}}\rangle, \tag{3}$$

where $|\varphi\rangle$ depends only on the electron coordinate, $|0_{\mathrm{ph}}\rangle$ represents the phonon's vacuum state with $a_{\mathbf{q}}|0_{\mathrm{ph}}\rangle = 0$, and $U|0_{\mathrm{ph}}\rangle$ is the coherent state of the phonon,

$$U = \exp\left[\sum_{\mathbf{q}}\left(a_{\mathbf{q}}^{+} f_q - a_{\mathbf{q}} f_q^*\right)\right], \tag{4}$$

where $f_q(f_q^*)$ is the variational function. We may choose the trial ground and the first-excited state wave functions of the electron to be

$$|\varphi_0\rangle = \left(\frac{2\lambda_0}{\pi}\right)\left(\frac{\mu_0}{\pi}\right)\exp\left[-\frac{\lambda_0\rho^2}{2}\right]\exp\left[-\frac{\mu_0 z^2}{2}\right], \tag{5}$$

$$|\varphi_1\rangle = 2\left(\frac{\lambda_1}{\pi}\right)^{1/2}\frac{\mu_1^{3/4}}{\pi^{1/4}}\exp\left(-\frac{\lambda_1\rho^2}{2}\right)\exp\left(-\frac{\mu_1 z^2}{2}\right)z, \tag{6}$$

where λ_0, μ_0, λ_1, and μ_1 are the variational parameters. Equations (5) and (6) satisfy the following normalized relations:

$$\langle\varphi_0|\varphi_0\rangle = 1, \quad \langle\varphi_0|\varphi_1\rangle = 0, \quad \langle\varphi_1|\varphi_1\rangle = 1. \tag{7}$$

By minimizing the expectation value of the Hamiltonian, we then obtain the polaron's ground state energy $E_0 = \langle\varphi_0|H|\varphi_0\rangle$ and the first excited state energy $E_1 = \langle\varphi_1|H|\varphi_1\rangle$. Choosing the usual polaron units ($\hbar = 2m = \omega_{\mathrm{LO}} = 1$), the ground state and the first-excited state energies of an electron in an AQD can be written as

$$E_0(\lambda_0, \mu_0) = \lambda_0 + \frac{\mu_0}{2} + \frac{1}{\lambda_0 l_1^4} + \frac{1}{2\mu_0 l_2^4} - \frac{\omega_{\mathrm{c}}^2}{16\lambda_0} - \alpha\sqrt{\frac{2\lambda_0}{\pi\,(1 - (\lambda_0/\mu_0))}}\arcsin\left(1 - \frac{\lambda_0}{\mu_0}\right)^{1/2}, \tag{8}$$

$$E_1(\lambda_1, \mu_1) = \lambda_1 + \frac{3\mu_1}{2} + \frac{1}{\lambda_1 l_1^4} + \frac{3}{2\mu_1 l_2^4} - \frac{\omega_c^2}{16\lambda_1} - \alpha\sqrt{\frac{2\lambda_1}{\pi(1-(\lambda_1/\mu_1))}}\arcsin\left(1-\frac{\lambda_1}{\mu_1}\right)^{1/2}, \tag{9}$$

where $l_1 = \sqrt{\hbar/m\omega_1}$, $l_2 = \sqrt{\hbar/m\omega_2}$ are respectively the transverse and longitudinal effective confinement lengths of the QD, and $\omega_c = eB/mc$ is the cyclotron frequency of a magnetic field. The transition frequency between the first excited and the ground states of the polaron is given by

$$\omega = \frac{E_1 - E_0}{\hbar}. \tag{10}$$

3. Numerical results and discussion

In this section, we calculate numerically the ground state energy E_0, the first excited state energy E_1, and the transition frequency ω of the polaron in an AQD under applied magnetic field along the z-direction. Choosing the usual polaron units ($\hbar = 2m = \omega_{LO} = 1$), the numerical results are given in figures 1, 2 and 3.

Figures 1–3 depict respectively E_0, E_1, and ω as functions of the cyclotron frequency of a magnetic field ω_c and the electron–phonon coupling strength α for $l_1 = 0.35$ and $l_2 = 0.45$. Figures 1–3 clearly illustrate that E_0, E_1, and ω are increasing functions of the cyclotron frequency ω_c. From the expression of $\omega_c = eB/mc$, one can see that

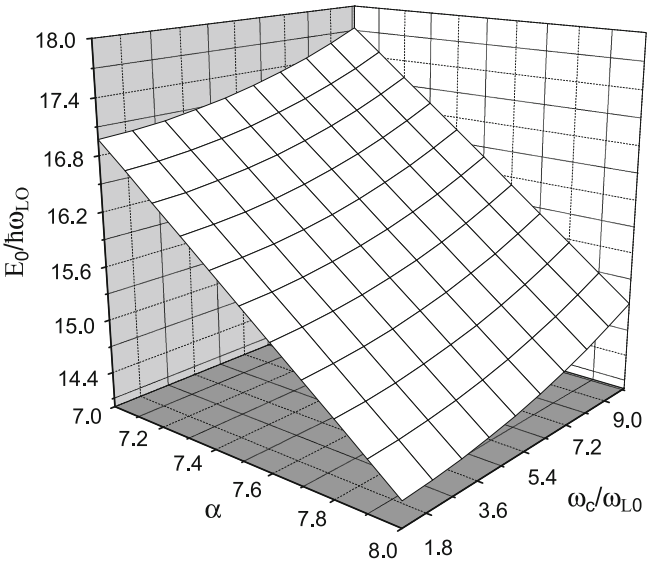

Figure 1. The relations of polaron's ground state energy E_0 with the electron–phonon coupling strength α and the cyclotron frequency ω_c for $l_1 = 0.35$ and $l_2 = 0.45$.

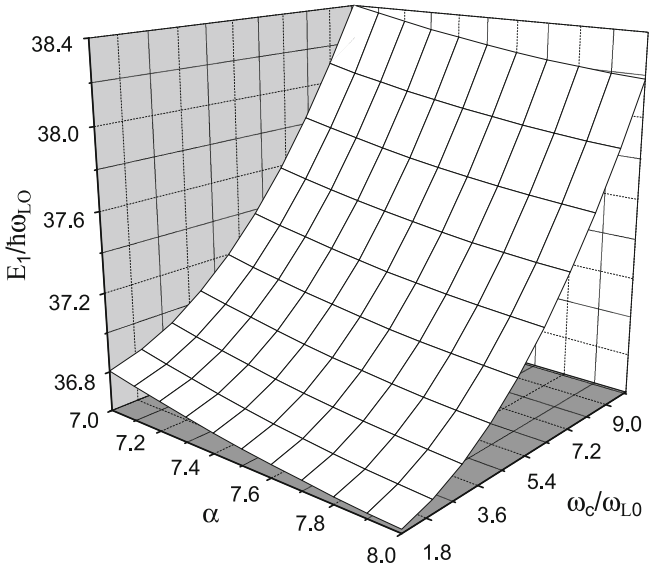

Figure 2. The relations of polaron's first excited state energy E_1 with the electron–phonon coupling strength α and the cyclotron frequency ω_c for $l_1 = 0.35$ and $l_2 = 0.45$.

E_0, E_1, and ω will increase by increasing the magnetic field B. The electron energy and the electron–phonon coupling energy increase with the increasing magnetic field. Therefore, E_0, E_1, and ω are enhanced. From another point of view, the presence the magnetic

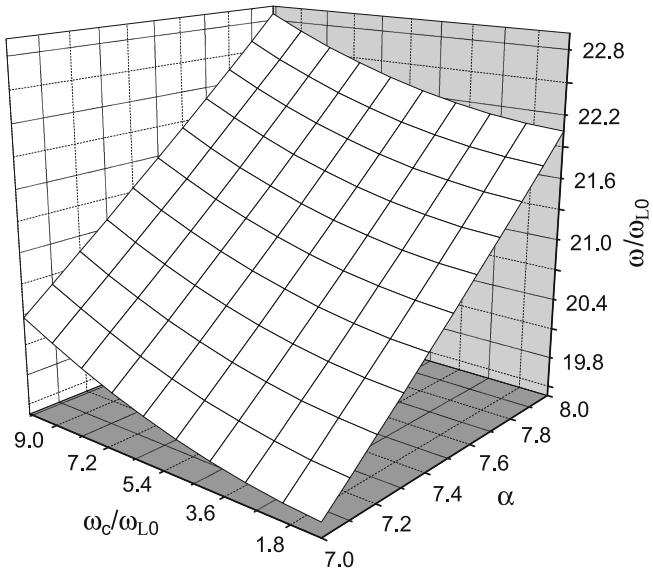

Figure 3. The relations of polaron's transition frequency ω with the electron–phonon coupling strength α and the cyclotron frequency ω_c for $l_1 = 0.35$ and $l_2 = 0.45$.

field is equivalent to the introduction of another new confinement on the electron, leading to greater electron wave function overlapping with each other. Thus, the electron energy, the electron–phonon interactions, the ground and the first excited state energies, and the transition frequency increase with increasing magnetic field. These results are in agreement with the results of Kandemir and Cetin [25], Vartanian *et al* [11], Nguyen *et al* [26] and ours [27] obtained respectively by using squeezed-state variational, adiabatic approximation, variational, and linear combination operator methods. We suggest a new way of tuning the AQDs state energies and the transition frequency by adjusting the magnetic field.

From figure 3, we can also see that the transition frequency ω is an increasing function of the electron–phonon coupling strength α. This is because the larger the electron–phonon coupling strength, the stronger is the electron–phonon interaction. Consequently, it leads to the increment of the electron's energy and makes the electron interact with more phonons, and the transition frequency of polaron in an AQD is increased. From figures 1 and 2, one can also see that the ground state energy and the first excited state energy are decreasing functions of the electron–phonon coupling strength α. The reason is that the last term in eqs (8) and (9) is respectively the contribution from the electron–phonon interaction term to the state energies, which is a negative value. As a result of this, the state energies of polaron in an AQD will increase with decreasing coupling strength. These results are in agreement with the results of Kandemir and Cetin [25], Lepine and Bruneau [28], Kandemir and Altanhan [29] and ours [17,27] obtained respectively by using squeezed-state variational, Fock approximation of Matz and Burkey, Lee–Low–Pines–Huybrechts variational, and linear combination operator methods. It is known that the electron–phonon coupling strength is different in different crystals. Thus, the state energies and the transition frequency of polaron in the AQDs can be tuned by changing it. We also suggest another way of tuning the AQDs state energies and the transition frequency by adjusting the electron–phonon coupling strength.

The research on a qubit consisting of a two-level system attracts the interest of many scholars [1–6]. In the present article, we have studied the ground and first excited state energies of an electron and the relevant eigenfunctions in an AQD, belonging to the basic research area of the two-level system and the results obtained by us may provide theoretical basis for the research of the relevant qubit.

4. Conclusion

Based on the Pekar-type variational method, which has different variational parameters in the x–y plane and the z-direction, we have calculated the ground and the first excited state energies as well as the transition frequency of the strong-coupling polaron in an AQD under an applied magnetic field along the z-direction. It is found that the ground and the first excited state energies and the transition frequency are increasing functions of external applied magnetic field. The ground state and the first excited state energies are decreasing functions of the electron–phonon coupling strength, whereas transition frequency is an increasing function of the electron–phonon coupling strength. We find two ways of tuning the AQD's state energies and the transition frequency: by adjusting (1) the magnetic field and (2) the electron–phonon coupling strength.

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