

Influence of an External Magnetic Field on Polaronic Properties in an Asymmetric Quantum Dot

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Received: 25.07.2025 & Accepted: 05.09.2025

Doi: [10.12693/APhysPolA.148.108](https://doi.org/10.12693/APhysPolA.148.108)

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An asymmetric quantum dot with shape anisotropy is selected as the theoretical model. By combining the linear combination operator method with the unitary transformation method, we theoretically derive an expression for the ground-state energy of a polaron in an asymmetric quantum dot, where this energy undergoes Zeeman splitting. In a weak magnetic field, the interaction between the spin magnetic moment and the magnetic field induces a splitting of the polaron energy into two components, with the Zeeman splitting energy being proportional to the magnetic field strength. The functional relationships between the ground-state energy and five critical parameters — the electron–phonon coupling strength, the vibration frequency, the magnetic field cyclotron resonance frequency, the transverse confinement length, and the longitudinal confinement length — are analyzed individually. The ground-state energy is an increasing function of the magnetic field cyclotron resonance frequency, while it is a decreasing function of the electron–phonon coupling strength, the vibration frequency, the transverse confinement length, and the longitudinal confinement length.

topics: asymmetric quantum dot, Zeeman effect, magnetic field, polaron

1. Introduction

With the continuous advancement and rapid evolution of material growth technologies, it has become feasible to fabricate semiconductor quantum dots with diverse morphologies. Quantum dots exhibit a number of novel optoelectronic properties and transport characteristics, which are significantly governed by electron–phonon coupling. As such, research on polaron-related phenomena in quantum dots has attracted extensive interest within the scientific community. In fact, numerous studies have investigated the impact of polarons on quantum dots. These studies include research on polaron-related topics in symmetric quantum dots [1–3], as well as investigations on the properties of polarons in asymmetric quantum dots with shape anisotropy. In anisotropic quantum dots, electrons are confined differently along different directions, most notably exhibiting distinct confinement strengths in the transverse and longitudinal dimensions. Currently, asymmetric quantum dots have become a prominent research focus in materials science and condensed matter physics. Exploring

their physical properties and applications necessitates both the development of sensitive experimental techniques [4–6] and in-depth advancement of theoretical analysis methodologies. For example, Lepine et al. [7] used the Fock approximation put forward by Matz and Burkey to examine the impact of asymmetric parabolic potentials on the ground-state energy of polarons in parabolic quantum dots. Kandemir et al. [8] adopted a trial wavefunction approach, which consists of the product of the electron wavefunction and the coherent phonon wavefunction, to study the polaron effect for low-energy electrons in asymmetric quantum dots. These dots are bound by a three-dimensional asymmetric harmonic potential in a magnetic field and further confined by a hydrogen-like impurity. Chen et al. [9] used the Feynman path integral approach to study the ground-state energy of electrons in asymmetric quantum dots that are simultaneously coupled to both the Coulomb potential and the longitudinal optical phonon field. Sako et al. [10] applied the quantum chemical configuration interaction method to calculate the spectra, electron density distributions, and ground-state correlation energies of two electrons confined in quantum dots, which are

subject to anisotropic harmonic oscillator potentials with different confinement strengths. Using a trial wavefunction approach constructed from the direct product of the electron and coherent phonon wavefunctions, Kandemir and Çetin [8] explored the polaron effect exhibited by low-lying electrons in asymmetric quantum dots. These dots are bound by a three-dimensional asymmetric harmonic potential in a magnetic field and additionally confined by a hydrogenic impurity.

Research on asymmetric quantum dots has progressed at a remarkable pace, solidifying its position as a compelling frontier in the science and technology of low-dimensional materials. However, research on the properties of the magnetic polaron in asymmetric quantum dots using the linear combination operator method remains scarce — in particular, the Zeeman effect of a polaron in such systems has yet to be explored. In this study, we will utilize the linear combination operator method to analyze the simple Zeeman effect of a polaron in an asymmetric quantum dot.

2. Theoretical model and theoretical derivation

In this work, we employ an asymmetric parabolic quantum dot as a theoretical model, wherein an electron is subjected to strong confinement potentials in three-dimensional space. The expression for such potentials is given as

$$V(r) = \frac{1}{2} m^* \omega_1^2 \rho^2 + \frac{1}{2} m^* \omega_2^2 z^2. \quad (1)$$

In (1), ω_1 and ω_2 represent the transverse confinement strength and the longitudinal confinement strength, respectively, while m^* stands for the electron's effective mass, and $r(\rho, z)$ denotes the electron's position vector. In the present model, we solely consider the Fröhlich interaction between the electron and the bulk longitudinal optical (LO) phonon field. Furthermore, a uniform magnetic field $\mathbf{B} = (0, 0, B)$ is applied along the z -direction, with the corresponding vector potential $\mathbf{A} = \frac{B}{2}(-y, x, 0)$ obeying the symmetric gauge. In the effective mass approximation, the full Hamiltonian of the system may be written as

$$\hat{H} = \hat{H}_e + \hat{H}_{ph} + \hat{H}_{e-ph} + \hat{H}_z. \quad (2)$$

In this context, the electronic term is expressed as

$$\hat{H}_e = \frac{1}{2m^*} \left(\mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 + V(r). \quad (3)$$

The phonon field term is formulated within the standard bosonic representation, i.e.,

$$\hat{H}_{ph} = \sum_{\mathbf{q}} \hbar \omega_{\text{LO}} \hat{a}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}}. \quad (4)$$

Here, ω_{LO} stands for the bulk longitudinal optical phonon frequency, $\mathbf{q}$ denotes the wave vector, while $\hat{a}_{\mathbf{q}}^\dagger$ and $\hat{a}_{\mathbf{q}}$ represent the phonon creation and

annihilation operators, respectively. The electron-phonon interaction term is given by

$$\hat{H}_{e-ph} = \sum_{\mathbf{q}} \frac{V_{\mathbf{q}}}{\sqrt{V}} \left(\hat{a}_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} + \hat{a}_{\mathbf{q}}^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}} \right). \quad (5)$$

In (5), V refers to the normalized volume, while $V_{\mathbf{q}}$ — the Fröhlich coupling constant — is formulated as

$$V_{\mathbf{q}} = i \left(\frac{\hbar \omega_{\text{LO}}}{q} \right) \left(\frac{\hbar}{2m^* \omega_{\text{LO}}} \right)^{1/4} (4\pi\alpha)^{1/2}, \quad (6)$$

where α denotes the electron-phonon coupling strength.

The Zeeman effect term is given by

$$\hat{H}_z = \frac{1}{2} g \mu_B B \hat{\sigma}_z. \quad (7)$$

Herein, g denotes the Landé factor, μ_B represents the Bohr magneton, and $\hat{\sigma}_z$ stands for the Pauli matrix operator.

We introduce linear combinations of operators for the electron's momentum and position coordinates, respectively, as

$$\hat{p}_j = \left(\frac{m^* \hbar \lambda}{2} \right)^{1/2} (\hat{b}_j + \hat{b}_j^\dagger), \quad (8)$$

and

$$\hat{r}_j = i \left(\frac{\hbar}{2m^* \lambda} \right)^{1/2} (\hat{b}_j - \hat{b}_j^\dagger), \quad (9)$$

for $j = x, y, z$. In this context, λ — variational parameter — denotes the oscillation frequency of the polaron. We perform a unitary transformation on the Hamiltonian of the system, with the unitary transformation operator given by

$$U = \exp \left[\sum_{\mathbf{q}} (\hat{a}_{\mathbf{q}}^\dagger f_{\mathbf{q}} - \hat{a}_{\mathbf{q}} f_{\mathbf{q}}^*) \right]. \quad (10)$$

Within the formula, $f_{\mathbf{q}}$ and $f_{\mathbf{q}}^*$ are variational parameters, derivable by minimizing the energy through variation. Following the unitary transformation, the system's Hamiltonian assumes the form

$$\begin{aligned} \hat{H}' = & \frac{1}{2m^*} \left[\left(p_x - \frac{\beta^2}{4} \hat{y} \right)^2 + \left(\hat{p}_y + \frac{\beta^2}{4} \hat{x} \right)^2 \right] + \frac{m^* \omega_1^2}{2} \hat{\rho}^2 \\ & + \frac{m^* \omega_2^2}{2} \hat{z}^2 + \sum_{\mathbf{q}} \hbar \omega_{\text{LO}} (\hat{a}_{\mathbf{q}}^\dagger + f_{\mathbf{q}}^*) (\hat{a}_{\mathbf{q}} + f_{\mathbf{q}}) \\ & + \sum_{\mathbf{q}} \frac{V_{\mathbf{q}}}{\sqrt{V}} \left[(\hat{a}_{\mathbf{q}} + f_{\mathbf{q}}) e^{i\mathbf{q} \cdot \mathbf{r}} + (\hat{a}_{\mathbf{q}}^\dagger + f_{\mathbf{q}}^*) e^{-i\mathbf{q} \cdot \mathbf{r}} \right] \\ & + \frac{1}{2} g \mu_B B \hat{\sigma}_z. \end{aligned} \quad (11)$$

Here, $\beta^2 = \frac{2eB}{c}$. We take the trial wavefunction for the system's ground state as

$$|\Psi_0\rangle = (\hat{a} \chi_{1/2} + \hat{b} \chi_{-1/2}) |0\rangle_a |0\rangle_b. \quad (12)$$

Here, $|0\rangle_b$ denotes the vacuum state of the operator $\hat{b}$, whereas $|0\rangle_a$ refers to the unperturbed zero-phonon state, satisfying $\hat{b}_j |0\rangle_b = \hat{a}_{\mathbf{q}} |0\rangle_a = 0$. In turn, $\chi_{1/2} = (1, 0)^T$ and $\chi_{-1/2} = (0, 1)^T$ correspond to the upward-split and downward-split

states, respectively. Substituting $\hat{\rho}_j$ and $\hat{r}_j$ into (12) and operating on the trial ground-state wavefunction, we derive the expectation value of the system's energy as

$$\begin{aligned} F(f_q, f_q^*) &= \frac{3\hbar\lambda}{4} + \frac{\beta^4\hbar}{32(m^*)^2\lambda} + \frac{\hbar\omega_1^2}{2\lambda} + \frac{\hbar\omega_2^2}{4\lambda} \\ &+ \sum_q \frac{1}{\sqrt{V}} (V_q f_q + V_q^* f_q^*) \exp\left(-\frac{\hbar q^2}{4m^*\lambda}\right) \\ &+ \sum_q \hbar\omega_{\text{LO}} |f_q|^2 \pm \frac{1}{2} g\mu_B B. \end{aligned} \quad (13)$$

Since $\frac{\partial F}{\partial f_q} = 0$, it follows that

$$f_q^* = -\frac{V_q \exp\left(-\frac{\hbar q^2}{4m^*\lambda}\right)}{V \hbar\omega_{\text{LO}}}. \quad (14)$$

By parity of reasoning, we obtain

$$f_q = -\frac{V_q^*}{V \hbar\omega_{\text{LO}} \exp\left(-\frac{\hbar q^2}{4m^*\lambda}\right)}. \quad (15)$$

Substituting f_q and f_q^* back into (13) and replacing summation by integration, we yield the polaron's ground-state energy

$$\begin{aligned} E &= \frac{3\hbar\lambda}{4} + \frac{\beta^4\hbar}{32m^2\lambda} + \frac{\hbar\omega_1^2}{2\lambda} + \frac{\hbar\omega_2^2}{4\lambda} - \alpha \hbar\omega_{\text{LO}} \sqrt{\frac{\lambda}{\pi\omega_{\text{LO}}}} \\ &\pm \frac{1}{2} g\mu_B B. \end{aligned} \quad (16)$$

As is apparent from (16), the ground-state energy of the polaron exhibits splitting. This phenomenon corresponds to the simple Zeeman effect, which arises from the interaction between the orbital magnetic moment and the magnetic field, assuming weak magnetic field conditions. It is also found from (16) that the Zeeman splitting energy is independent of the electron-phonon coupling strength. Based on the Zeeman effect theory, Zeeman splitting originates from the energy correction induced by the varying projections of the total atomic angular momentum along the direction of an external magnetic field. Notably, the Zeeman splitting energy depends largely on the magnetic moment of the atoms and the external magnetic field intensity, and bears no direct relation to the electron-phonon coupling strength. Consequently, the above conclusion is obtained on the basis of our theoretical derivation.

Herein, the magnetic field cyclotron resonance frequency is given by $\omega_c = \frac{eB}{m^*c}$, the transverse and longitudinal confinement lengths are defined as $l_1 = \sqrt{\hbar/(m^*\omega_1)}$ and $l_2 = \sqrt{\hbar/(m^*\omega_2)}$, respectively, the Bohr magneton is $\mu_B = e\hbar/(2m_0c)$, and $\gamma = mg/(2m_0)$. We work with the polaron units $\hbar = \omega_{\text{LO}} = 2m^* = 1$. The ground-state energy of the polaron transforms to

$$E = \frac{3}{4}\lambda + \frac{\omega_c^2}{8\lambda} + \frac{2}{\lambda l_1^4} + \frac{1}{\lambda l_2^4} - \alpha \sqrt{\frac{\lambda}{\pi}} \pm \frac{1}{2} \gamma \omega_c. \quad (17)$$

3. Numerical calculations and discussion of results

The ground-state energy of the polaron has been derived by theoretical deduction. It is shown that the ground-state energy depends on the vibration frequency, the magnetic field cyclotron frequency, the transverse and longitudinal confinement lengths, and the electron-phonon coupling strength. To visually illustrate the influence of the Zeeman effect on the ground-state energy of the polaron in an asymmetric parabolic quantum dot, we perform numerical calculations on the ground-state energy of the polaron. We separately discuss the variation relationships between the ground-state energy and, respectively, the vibration frequency λ , the magnetic field cyclotron resonance frequency ω_c , the electron-phonon coupling strength, the transverse confinement length l_1 , and the longitudinal confinement length l_2 . The results of the calculations are presented in Figs. 1–5. In each figure, E_0 denotes the ground-state energy of the polaron without taking into account the Zeeman effect, E_+ represents the upward-split energy of the polaron when the Zeeman effect is taken into account, and E_- stands for the downward-split energy of the polaron when the Zeeman effect is taken into account.

Figure 1 illustrates the variation of the polaron ground-state energy E with the vibration frequency λ and the electron-phonon coupling strength α , provided that $l_1 = 0.3$, $l_2 = 0.5$, $\omega_c = 5$, and $\gamma = 2$ are fixed. The solid line denotes the polaron ground-state energy E_0 without considering the Zeeman effect, whereas the short solid line and the dotted line represent the upward-split energy E_+ and downward-split energy E_- of a polaron, respectively, when the Zeeman effect is included in the analysis. Figure 1 reveals that the polaron ground-state energy curve exhibits a decaying trend with increasing vibration frequency. In the expression (17) for the ground-state energy, not only is the electron kinetic energy related to the vibration frequency, but the magnetic field energy, electron-phonon interaction energy, and confinement potential energy are also associated with λ . The contribution of the vibration frequency to the electron kinetic energy is positive. However, the vibration frequency is inversely proportional to both the magnetic field energy and the confinement potential energy, and its contribution to the electron-phonon interaction energy is negative. From the trend of the curves in the figure, it can be seen that the contribution of the vibrational frequency to the magnetic field energy, electron-phonon interaction energy, and confinement potential energy is greater than to the kinetic energy of the electron. When the vibrational frequency is around $\lambda = 2$, the polaron ground-state energy is weakly influenced by the electron-phonon coupling strength. As the vibrational frequency increases, the spacing between the curves

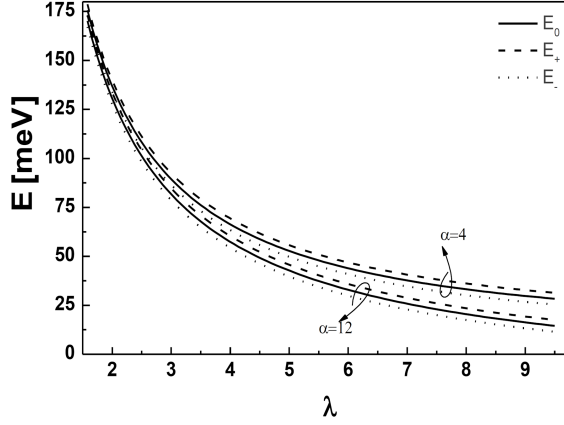


Fig. 1. Curves showing the relationship between the ground-state energy E and the vibration frequency λ for different values of the electron-phonon coupling strength α .

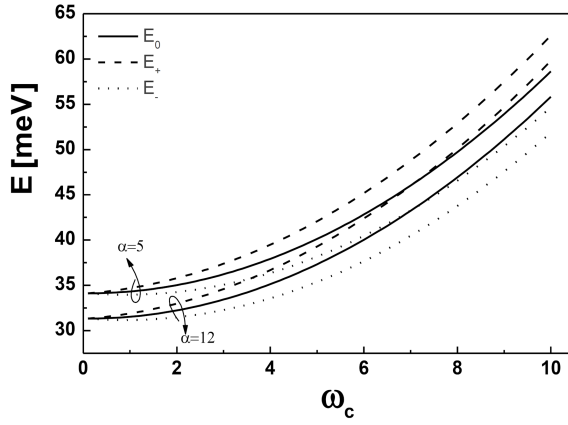


Fig. 2. Curves showing the relationship between the ground-state energy E and the magnetic field cyclotron resonance frequency ω_c for different values of the electron-phonon coupling strength α .

widens progressively, which indicates that the interaction between the electron and its surrounding phonons increases with increasing vibrational frequency. It is also observed in Fig. 1 that the ground-state energy of the polaron splits into two branches (upper and lower). This occurs because the Zeeman effect causes the ground-state energy of the polaron to split in a magnetic field.

With the fixed parameters set as $l_1 = 0.6$, $l_2 = 0.8$, $\lambda = 0.5$, and $\gamma = 0.8$, Fig. 2 demonstrates the functional dependence of the polaron ground-state energy on (i) the cyclotron resonance frequency in a magnetic field and (ii) the electron-phonon coupling strength. The solid line denotes the ground-state energy E_0 of the polaron without considering the Zeeman effect, whereas the short solid line and the dotted line represent the upward-split energy E_+ and downward-split energy E_- of the polaron, respectively, when the Zeeman effect is

taken into account. As can be seen in Fig. 2, the polaron ground-state energy exhibits a parabolic increase with increasing the cyclotron resonance frequency ω_c , which indicates that the polaron ground-state energy is an increasing function of ω_c . The expression $\omega_c = \frac{eB}{mc}$ is proportional to the magnetic field B , and so grows with B . As the magnetic field increases, the electron wavefunctions have a larger overlap with the phonon wavefunction, leading to an increase in the magnetic field energy of the polaron. In the expression (17) for the polaron ground-state energy, assuming that the magnetic field energy makes a positive contribution to the ground-state energy, the latter increases with the former. Since the magnetic field energy is proportional to the square of the magnetic field cyclotron resonance frequency, this trend manifests itself in a parabolic shape. From Fig. 2, it is further observed that the polaron ground-state energy splits into two branches. This splitting arises from the Zeeman effect under the influence of a magnetic field. As ω_c increases, the energy splitting gap widens. This can be explained the last term of (17), because the magnetic field cyclotron resonance frequency is proportional to the Zeeman splitting energy. When $\omega_c = 0$, the energy splitting vanishes, indicating the absence of the Zeeman effect at zero magnetic field.

It can also be seen from Figs. 1 and 2 that when the vibrational frequency (or the magnetic field cyclotron resonance frequency) is fixed, the stronger the electron-phonon interaction, the smaller the ground-state energy of the polaron. In (17), the electron-phonon coupling strength α has a negative contribution to the polaron ground-state energy. Hence, the stronger the electron-phonon coupling, the lower the polaron energy. The presence of phonons lowers the energy of the polaron. As a result, the polaron state is more stable than the bare electron state, and this stability in turn enhances the stability of the polaron energy splitting.

For $l_2 = 0.6$, $\lambda = 0.2$, $\omega_c = 2$, $\alpha = 14$, and $\gamma = 1.0$, Fig. 3 demonstrates the functional relationship between the ground-state energy E of the polaron and the transverse confinement length l_1 . In turn, Fig. 4 demonstrates the dependence between the ground-state energy E of the polaron and the longitudinal confinement length l_2 , when $l_1 = 0.5$, $\lambda = 0.2$, $\omega_c = 2$, $\alpha = 8$, and $\gamma = 1.0$. From the relationship between confinement length and confinement strength, respectively given by $l_1 = \sqrt{\hbar}/(m^* \omega_1)$ and $l_2 = \sqrt{\hbar}/(m^* \omega_2)$, it can be seen that the confinement length is inversely proportional to the square root of the confinement strength. An increase in the confinement length implies a decrease in the confinement strength, i.e., the binding effect of the quantum dot on the electrons weakens. The weakening of the quantum confinement effect reduces the electron binding energy, while the contribution of the electron-phonon interaction further reinforces this trend. As the

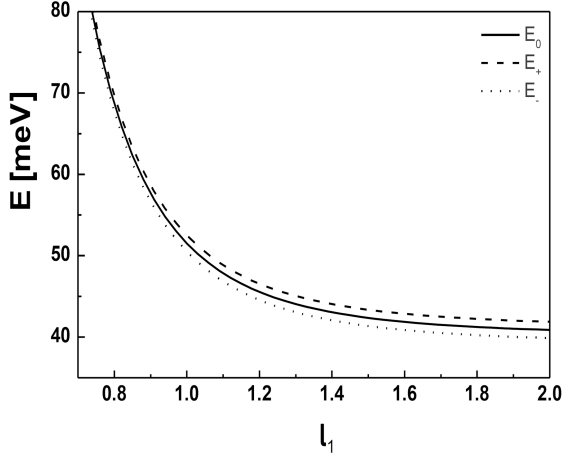


Fig. 3. Curve of the relationship between the ground-state energy E and the lateral confinement length l_1 under the Zeeman effect.

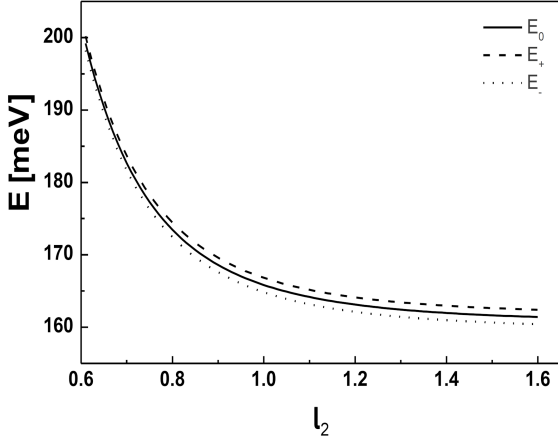


Fig. 4. Curve of the relationship between the ground-state energy E and the longitudinal confinement length l_2 under the Zeeman effect.

confinement length increases, the negative contribution of this electron-phonon interaction energy becomes even more pronounced. Note that as the confinement length increases, the confining potential energy decreases, while the negative contribution of the electron-phonon interaction increases more strongly. These two factors collectively cause an overall reduction in the polaron ground-state energy. This conclusion reflects the quantum confinement effect, specifically that the smaller the confinement length, the greater the polaron ground-state energy.

For $\lambda = 1.0$, $l_1 = 1.0$, $l_2 = 1.2$, $\alpha = 10$, and $\gamma = 2$, Fig. 5 shows the variation law of the ratio of the polaron ground-state energy to the Zeeman splitting energy, E_0/E_Z , with the magnetic field cyclotron resonance frequency ω_c and the electron-phonon coupling strength α . As is evident in Fig. 5, regardless of the value assigned to α , the ratio

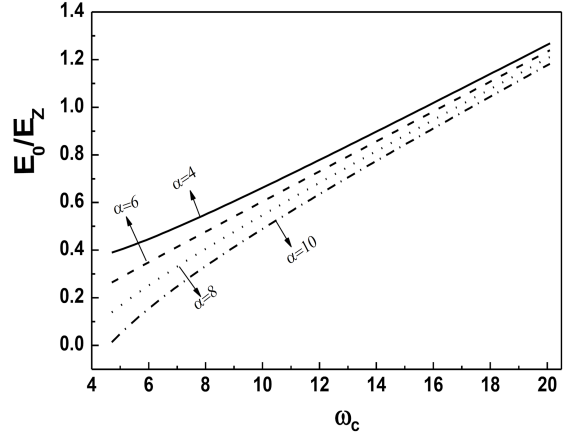


Fig. 5. Curves of the ratio of zero-field splitting energy to Zeeman splitting energy, E_0/E_Z , as a function of the magnetic field cyclotron resonance frequency ω_c for different values of the electron-phonon coupling strength α .

E_0/E_Z increases as ω_c increases. The phenomenon whereby the ratio E_0/E_Z increases with ω_c arises essentially from the discrepancy in their rates of change with magnetic-field strength. From the trend of the curves, it is seen that the magnitude of the increase in the ground-state energy outpaces that of the Zeeman splitting energy. The Zeeman splitting energy E_Z is in a linear positive correlation with the magnetic field cyclotron resonance frequency ω_c . The case of the polaron ground-state energy E_0 is different, since the square of the magnetic cyclotron resonance frequency contributes positively to E_0 . Thus, as ω_c increases, E_0 grows at a faster than linear rate. When ω_c is fixed, a comparison of curves for different electron-phonon coupling strength shows that the stronger the electron-phonon coupling strength, the higher the ratio of the polaron ground-state energy to the Zeeman splitting energy. The stronger the electron-phonon coupling strength, the more intense the electron-phonon interaction, leading to a more significant negative contribution to the ground-state energy. But, even as the magnetic field increases, localized electrons dampen this negative contribution. In systems with stronger electron-phonon coupling α , this dampening effect exerts a more notable impact on the total energy. This is equivalent to an additional increase in the polaron ground-state energy. The Zeeman splitting energy is mainly governed by the electron spin magnetic moment and the magnetic field — with no direct connection to the electron-phonon coupling strength. Therefore, the stronger the electron-phonon coupling strength, the more distinct the growth advantage of the ground-state energy over the Zeeman splitting energy. This ultimately results in the overall E_0/E_Z curve being higher as the electron-phonon coupling strength increases.

4. Conclusions

Using a combination of the linear combination operator method and the unitary transformation method, we theoretically derive the expression for the ground-state energy of a polaron in an asymmetric quantum dot under the influence of the Zeeman effect. In a weak magnetic field, the spin magnetic moment interacts with the magnetic field, inducing splitting of the polaron energy into two components. The Zeeman splitting energy is proportional to the magnetic field strength. As the cyclotron resonance frequency increases, the energy splitting interval widens accordingly. In the absence of a magnetic field, the energy levels remain degenerate, confirming the absence of the Zeeman effect under such conditions. Functional relationships between the ground-state energy and the electron-phonon coupling strength, the vibration frequency, the magnetic field cyclotron resonance frequency, the transverse confinement length, and the longitudinal confinement length are discussed. The ground-state energy is an increasing function of the magnetic field cyclotron resonance frequency, whereas it behaves as a decreasing function with respect to the electron-phonon coupling strength, the vibration frequency, the transverse confinement length, and the longitudinal confinement length.

Acknowledgments

This work was supported by Key Scientific and Technological Research Project of Liaoning Provincial Department of Education (Grant No. LJKZZ202200547).

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