Magnetic field and temperature dependence of the ground-state energy of weak-coupling magnetopolaron in quantum rods with hydrogenic impurity*

XIAO Xin(肖欣)[1], **Wuyunqimuge**(乌云其木格)[2], **HAN Chao**(韩超)[1], **and Eerdunchaolu**(额尔敦朝鲁)[1**]
1. Institute of Condensed Matter Physics, Hebei Normal University of Science & Technology, Qinhuangdao 066004,China
2. College of Physics and Electronic Information, Inner Mongolia University for Nationalities, Tongliao 028043, China

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The dependence of the ground-state properties of weak-coupling bound magnetopolarons in quantum rods (QRs) with hydrogenic impurity on magnetic field and temperature is studied by means of the Lee-Low-Pines (LLP) transformation method and Huybrechts linear combination operator method. The expression for the ground-state energy of the magnetopolaron is derived. Results of the numerical calculations show that the ground-state energy of weak-coupling bound magnetopolarons in QRs with hydrogenic impurity increases with increasing the cyclotron frequency of the magnetic field, the confinement strength of QRs and the temperature, but decreases with increasing the electron-phonon coupling strength and the dielectric constant ratio. The stability of the ground state of magnetopolarons is closely related to the aspect ratio e' of the QR. The ground state of magnetopolarons is the most stable at $e'=1$. The stability of the ground state of magnetopolarons can remarkably decrease when the value of the aspect ratio increases or decreases from 1.

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Many properties of quantum rods (QRs)[1-3] were investigated by means of the effective-mass envelope-function theoretical method, the semiempirical pseudopotential method[4], the eight-band effective-mass approximation method[5] and the configuration-interaction method[6], respectively, which involve the phonon effects. However, as most nanostructures are composed of the ionic crystals or the polar semiconductors, the electron-phonon coupling strongly affects their physical properties[7]. Therefore, the electron-phonon interaction in the QR has gradually been paid great attention. Comas et al[8] investigated the properties of the surface optical phonons in a semiconductor QR by using the theory based on the dielectric continuum approach method, and compared the results with that of the spherical quantum dot (QD) and quasi-spherical quantum dot. Xiao et al[9,10] studied the vibrational frequency and the ground-state binding energy of the strong-coupling magnetopolaron in a QR. For simplicity, the above works only discussed the case of 0 K. However, the thermal properties of the electron-phonon interaction system in QRs have rarely been studied so far. Especially, the influence of the magnetic field and the lattice thermal vibration on the properties of the weak-coupling bound magnetopolaron in QRs with impurity has never been investigated yet. In fact, these have a practical significance for improving the photoelectric properties of devices. In this paper, the magnetic field and temperature dependence of the properties of the ground-state of weak-coupling bound magnetopolaron in QRs with hydrogenic impurity is studied by means of the Lee-Low-Pines (LLP) transformation method, the Huybrechts linear combination operator method and the quantum statistical theory.

It is assumed that the electron is bound in the hydrogenic impurity, and interacts with the longitudinal optical (LO) phonon field. The electron is confined by different parabolic potentials in the x-y plane and the z position, respectively. The impurity atom is taken as the coordinate origin, and the electron is in a constant magnetic field $\boldsymbol{B}=(0, 0, B)$, which is perpendicular to the motion plane, so the Hamiltonian of the impurity-electron-phonon system in the QR can be written as:

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** E-mail: eerdunchaolu@163.com

$$H=\frac{1}{2m}\left(p_x-\frac{\beta^2}{4}y\right)^2+\frac{1}{2m}\left(p_y+\frac{\beta^2}{4}x\right)^2+\frac{p_z^2}{2me'^2}+\frac{1}{2}m\omega_\parallel{}^2\boldsymbol{\rho}^2+\frac{e'^2}{2}m\omega_z^2z^2-\frac{e^2}{\varepsilon_\infty|\boldsymbol{r}'|}+\sum_{\boldsymbol{q}}\hbar\omega_{\mathrm{LO}}b_{\boldsymbol{q}}^+b_{\boldsymbol{q}}+\sum_{\boldsymbol{q}}\left(V_{\boldsymbol{q}}b_{\boldsymbol{q}}\,\mathrm{e}^{\mathrm{i}(\boldsymbol{q}_\parallel\cdot\boldsymbol{\rho}+e'q_zz)}+h.c.\right)\ ,\tag{1}$$

where the first three terms represent the electronic kinetic energy, the fourth and fifth terms are the parabolic potential of the QR, the sixth term is the Coulomb bound potential, the seventh term is the phonon energy, and the last term represents the electron-LO-phonon interaction. m, $\boldsymbol{r}=(\boldsymbol{\rho}, z)$ and $\boldsymbol{p}$ represent the mass, coordinate and momentum of the electron, respectively. $\omega_\parallel$ and ω_z are the transverse and longitudinal confinement frequencies. $b_q^+(b_q)$ is the creation (annihilation) operator of a bulk LO phonon with wave vector of $\boldsymbol{q}=(\boldsymbol{q}_\parallel, q_z)$. $e'=L/2R$ is the aspect ratio of the QR, where L is the longitudinal length of the QR, and R is the transverse radius of the QR, $\beta^2=2eB/c$.

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

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

where γ is the volume of the crystal, α is the electron-phonon coupling strength, and $\varepsilon_\infty(\varepsilon_0)$ is the high-frequency (static) dielectric constant.

First, the Coulomb potential is expanded as a series,

$$-\frac{e^2}{\varepsilon_\infty|\boldsymbol{r}'|}=-\frac{4\pi e^2}{\varepsilon_\infty v}\sum_{\boldsymbol{q}}\frac{1}{q^2}\exp[-\mathrm{i}(\boldsymbol{q}_\parallel\cdot\rho+e'q_zz)]\ .\tag{3}$$

To discuss the effective Hamiltonian of the impurity bound magnetopolaron in the QR, the Huybrechts linear combination operator is introduced into the momentum and coordinate of the electron[11],

$$p_j=\left(\frac{m\hbar\lambda}{2}\right)^{\frac{1}{2}}(a_j+a_j^+),\ \ r_j=\mathrm{i}\left(\frac{\hbar}{2m\lambda}\right)^{\frac{1}{2}}(a_j-a_j^+),(j=x,y,z)\ ,\tag{4}$$

where λ is variational parameter. Then we discuss the expectation value of the operator function $U_2^{-1}U_1^{-1}HU_1U_2$ in the state $|\psi\rangle$, so it is obtained that

$$\overline{H}=\langle\psi|U_2^{-1}U_1^{-1}HU_1U_2|\psi\rangle\ ,\tag{5}$$

where

$$U_1=\exp\left(-\mathrm{i}\,A\sum_{\boldsymbol{q}}(\boldsymbol{q}_\parallel\cdot\boldsymbol{\rho}+e'q_zz)b_{\boldsymbol{q}}^+b_{\boldsymbol{q}}\right)\ ,$$

$$U_2=\exp\left(\sum_{\boldsymbol{q}}(f_{\boldsymbol{q}}b_{\boldsymbol{q}}^+-f_{\boldsymbol{q}}^*b_{\boldsymbol{q}})\right)\ ,\tag{6}$$

are LLP unitary transformations[12], and $f_q(f_q^*)$ is the variational parameter. A characterizes the strength of the electron-phonon coupling. For the electron-phonon weak-coupling case, A=1[11,12].

$$|\psi\rangle=|\phi(z)\rangle|\{n_{\boldsymbol{q}}\}\rangle|\{n_j\}\rangle\ ,\tag{7}$$

is the trial wave function of the system under the finite temperature, where $\phi(z)$ is the wave function of the electron in z direction, which satisfies $\langle\phi(z)|\phi(z)\rangle=1\cdot|\{n_{\boldsymbol{q}}\}\rangle$ is the phonon state, and $|\{n_j\}\rangle$ is the polaron state. According to Ref.[13], the mean number of the electrons and the phonons can approximately be used to replace the number of them. According to the quantum statistical theory,

$$\overline{n}_{\boldsymbol{q}}=[\exp(\gamma)-1]^{-1},\overline{n}=[\exp(\gamma\lambda/\omega_{\mathrm{Lo}})+1]^{-1}\ ,\tag{8}$$

where $\gamma=\hbar\omega_{\mathrm{LO}}/k_{\mathrm{B}}T$ is the temperature parameter, k_{B} is the Boltzmann constant, and T is the thermo-dynamic temperature. Substituting Eqs.(1)-(4) and (6)-(8) into Eq.(5), the expectation value $\overline{H}$ can be obtained as

$$\overline{H}=\langle\phi(z)|F(f_{\boldsymbol{q}},f_{\boldsymbol{q}}^*,\lambda)|\phi(z)\rangle\ ,\tag{9}$$

where $F(f_q,f_q^*,\lambda)$ is called the variational function. The variational extreme value H_{eff} to $f_q(f_q^*)$ and λ is called the effective Hamiltonian of the system, which can be described as

$$H_{\mathrm{eff}}=\lim F(f_{\boldsymbol{q}},f_{\boldsymbol{q}}^*,\lambda)=\sum_{\boldsymbol{q}}\overline{n}_{\boldsymbol{q}}\hbar\omega_{\mathrm{LO}}+E_0\ ,\tag{10}$$

where

$$E_0=\frac{\hbar\lambda}{4}\left(2+\frac{1}{e'^2}\right)(2\overline{n}+1)+\frac{\hbar}{4\lambda}\left(2\omega_\parallel^2+e'^2\omega_z^2+\frac{\omega_c^2}{2}\right)(2\overline{n}+1)-\frac{\alpha\hbar\omega_{\mathrm{LO}}}{(4\overline{n}_{\boldsymbol{q}}+1)^{1/2}}B(e')-\frac{2\alpha\hbar}{1-\eta}\sqrt{\frac{2\omega_{\mathrm{LO}}\lambda}{\pi}}(1-\overline{n})A(e')\ ,\tag{11}$$

is the ground-state energy of the magnetopolaron, where $\eta=\varepsilon_\infty/\varepsilon_0$ is the dielectric constant ratio, and $\omega_c=eB/mc$ is the cyclotron frequency of the magnetic field. $A(e')$ and $B(e')$ are the functions of e', which can be written as

$$A(e')=\begin{cases}\dfrac{1}{\sqrt{1-e'^2}}\arcsin\sqrt{1-e'^2}, & e'<1\\ 1, & e'=1\\ \dfrac{1}{2\sqrt{e'^2-1}}\ln\dfrac{e'+\sqrt{e'^2-1}}{e'-\sqrt{e'^2-1}}, & e'>1\end{cases}$$

$$B(e')=\begin{cases}\dfrac{e'}{2\sqrt{1-e'^2}}\ln\dfrac{1+\sqrt{1-e'^2}}{1-\sqrt{1-e'^2}}, & e'<1\\ 1, & e'=1\\ \dfrac{e'}{\sqrt{e'^2-1}}\arcsin\dfrac{\sqrt{e'^2-1}}{e'}, & e'>1\end{cases}.\tag{12}$$

It can be seen from Eq.(11) that the ground-state energy E_0 of the magnetopolaron consists of four parts. The first two terms express the contributions of the kinetic energy of electronic motion, the quantum size effect of the QR, the confinement strength and the magnetic field to the ground-state energy of the magnetopolaron, and the last two terms express the contributions of the electron-LO-phonon coupling and the Coulomb bound potential between the electron and the impurity to the ground-state energy of the magnetopolaron. It can be seen that the contributions of the former are positive, while those of the latter are negative. It is obvious that E_0 is related to the cyclotron frequency ω_c of the magnetic field, the temperature parameter γ, the aspect ratio e' of the QR, the dielectric constant ratio η, and the transverse and longitudinal confinement strength $\omega_{\parallel}$ and ω_z. It should be self-consistent with Eq.(8). To show the dependence of E_0 on e', $\omega_{\parallel}(\omega_z)$, η, ω_c and γ, the results of numerical calculations are shown in Figs.1-3, taking $\hbar\omega_{LO}$ as the unit of energy, and ω_{LO} as the unit of λ, $\omega_{\parallel}$, ω_z and ω_c.

Fig.1 shows the dependence of the ground-state energy E_0 of the weak-coupling impurity bound magnetopolaron on the aspect ratio e' of the QR at different coupling strengths α in the QR. From Fig.1, it can be seen that E_0 increases with decreasing e' when $e'<1$, but increases with increasing e' when $e'>1$. E_0 has a minimum value at $e'=1$. This result is similar to that in Ref.[13]. It shows that the stability of the ground state of the magnetopolaron remarkably decreases when QDs are elongated to ellipsoidal QRs, but the stability is the best only when QRs change into spherical QDs. This shows a novel quantum size effect of the QR. It can also be seen from Fig.1 that E_0 decreases with increasing α. This is because the contribution of the electron-phonon interaction to the energy of magnetopolarons is negative, which can be seen from Eq.(11), and thus the larger α means the stronger electron-phonon coupling, lower ground-state energy of magnetopolarons and more stable ground state of magnetopolaron.

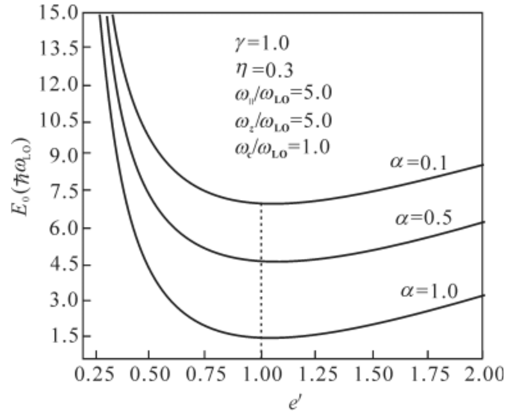

Fig.1 Ground-state energy E_0 versus the aspect ratio e' of the QR at different electron-phonon coupling strengths

Fig.2 shows the dependence of the ground-state energy E_0 of the magnetopolaron on the temperature parameter γ at different dielectric constant ratios η and cyclotron frequencies ω_c of the magnetic field. It can be seen from Fig.2 that E_0 decreases with increasing γ, in other words, with increasing the temperature T. The lattice thermal vibration is enhanced due to the increase of the temperature, so the number of phonons increases and an electron interacts with more phonons, which leads to the increase of the energy of magnetopolarons. It can also be seen that E_0 decreases with increasing η. It is because the contribution of the Coulomb bound potential between the electron and the impurity to the energy of magnetopolarons is negative, which can be seen from Eq.(11). The presence of the Coulomb potential is equivalent to another confinement on electrons, which leads to greater wave-function overlapping. Therefore, the increase of η means the increase of the Coulomb bound potential, which leads to the decrease of E_0. So the Coulomb bound potential makes the ground state of magnetopolarons more stable. It can also be seen from Fig.2 that E_0 increases with increasing the cyclotron frequency ω_c of the magnetic field. It shows that the external magnetic field enhances the electron-lattice polarization field, and thus enhances the three-body interaction of the electron-phonon-magnetic field in the QR.

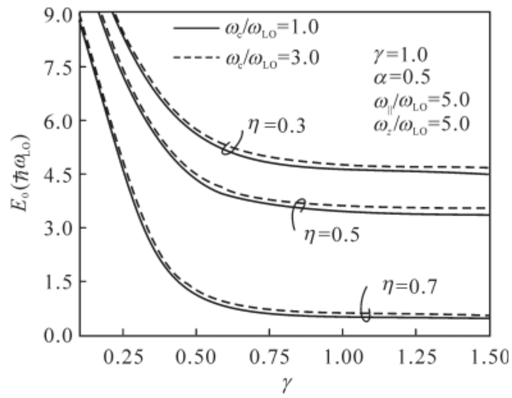

Fig.2 Ground-state energy E_0 versus the temperature parameter γ at different dielectric constant ratios η and cyclotron frequencies ω_c of magnetic field

Fig.3 shows the dependence of the ground-state energy E_0 of the magnetopolaron on the confinement strength $\omega_{\parallel}(\omega_z)$ at different aspect ratios e' of the QR. It can be seen from Fig.3 that E_0 increases with increasing $\omega_{\parallel}(\omega_z)$. It is because the presence of the transverse and longitudinal confinement potentials confines the electronic motion, leading to the increase of the electronic thermal-motion energy and the electron-phonon interaction, which take the phonons as the medium, due to the decrease of the range of the particle motion. It can also be seen from Fig.3 that the slopes of the curves increase with decreasing e'. It is another quantum size effect of the QR.

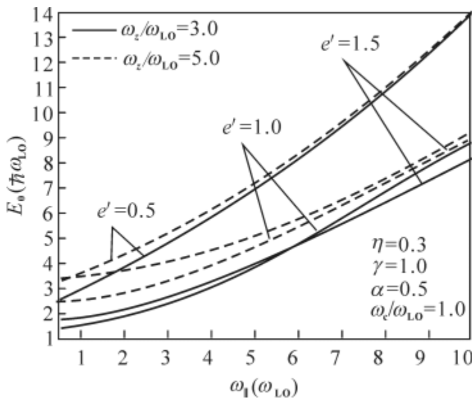

Fig.3 Ground-state energy E_0 versus the confinement strength $\omega_{\parallel}(\omega_z)$ at different aspect ratios e' of the QR

In conclusion, the ground-state energy of weak-coupling bound magnetopolarons in QRs with hydrogenic impurity increases with increasing the cyclotron frequency of the magnetic field, the confinement strength of QRs and the temperature, but decreases with increasing the electron-phonon coupling strength and the dielectric constant ratio. The stability of the ground state of magnetopolarons is closely related to the aspect ratio e' of the QR. The ground state of magnetopolarons is the most stable at e'=1. The stability of the ground state of magnetopolarons will remarkably decrease when the value of aspect ratio e' increases or decreases from 1.

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