Influence of temperature and LO phonon on the effective mass of bipolarons in polar semiconductor quantum dots*

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The temperature and LO phonon effects of the bipolaron in polar semiconductor quantum dots (QDs) are studied by using the Tokuda modified linear-combination operator method and the Lee-Low-Pines variational method. The expressions for the mean number of LO phonons and the effective mass of the bipolaron are derived. Numerical results show that the mean number of LO phonons of the bipolaron decreases with increasing the temperature and the relative distance r between two electrons, but increases with increasing the electron-phonon coupling strength α. The effective mass of the bipolaron M^* increases rapidly with increasing the relative distance r between two electrons when r is smaller, and it reaches a maximum at $r\approx 4.05r_p$, while after that, M^* decreases slowly with increasing r. The effective mass of the bipolaron M^* decreases with increasing the temperature. The electron-phonon coupling strength α markedly influences the changes of mean number of LO phonons and the effective mass M^* with the relative distance r and the temperature parameter γ.

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As most quantum dots (QDs)[1-3] structures are composed of ionic crystals or polar semiconductors, the electron-phonon coupling strongly influences their physical properties[4]. Therefore, the studies on some concrete problems, such as the influence of the phonon effects on the effective mass and the energy of electrons in QDs and so on, have aroused great interest in recent years. Xiao et al[5] studied the effective mass of polarons in semiconductor QDs by using the modified linear-combination operator method. Yin et al[6] investigated the effective mass and interaction energy of weak-coupling bound polarons in QDs by means of the linear-combination operator and unitary transformation methods. Xiao et al[7] discussed the effective mass of strong-coupling polarons in parabolic QDs on basis of the linear-combination operator method. One of the authors of this paper[8] used Tokuda linear-combination operator and Lee-Low-Pines transformation methods to research the influence of the temperature and the magnetic field on the ground-state energy and effective mass of the strong-coupling magnetopolaron in asymmetric parabolic QDs. Ge et al[9] studied the influence of the speed of polarons on the effective mass and the ground-state energy of magnetopolarons in QDs on the basis of linear-combination operator and unitary transformation methods considering the Rashba spin-orbit interaction. Li et al[10] researched the effective mass of the strong-coupling polaron in asymmetric QDs by using the Tokuda linear-combination operator and unitary transformation methods. Recently, Chen et al[11] investigated the effective mass of the strong-coupling magnetopolaron in parabolic QDs by means of the Landau-Pekar variational method. However, the phonon effects of the bipolaron which is formed by interaction between a pair of electrons and LO phonons, and the influence of that on the effective mass in QDs have never been concerned yet. In fact, two same electrons can form the bound state of the bipolaron through the interaction of the phonon field in the QD structure of ionic crystals or polar semiconductors[12]. Such study will be helpful to deeply understand the electron-phonon interaction in low-dimensional nanostructures. On the other hand, it is closely linked to the bipolaron mechanism of the high-temperature superconducting cuprate[13]. In this paper, the Tokuda modified linear-combination operator method and the Lee-Low-Pines variational method are used to study the effects of the temperature and the LO phonon on the effective mass and the mean number of LO phonons

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of bipolarons in polar semiconductor QDs.

The system of two electrons-LO phonon interaction in the QD is described by the following Frolich Hamiltonian[12]:

$$H=\frac{\boldsymbol{P}^2}{2M}+\frac{\boldsymbol{p}^2}{2\mu}+\frac{1}{2}M\Omega^2R^2+\frac{1}{2}\mu\Omega^2r^2+\frac{e^2}{\varepsilon_\infty r}+$$
$$\sum_k\hbar\omega_{\mathrm{LO}}a_k^+a_k+2\sum_k\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{r}}{2}\right)\left(v_ka_k\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}+v_k^*a_k^+\,\mathrm{e}^{-\boldsymbol{k}\cdot\boldsymbol{R}}\right)\ ,\qquad(1)$$

where $\boldsymbol{R}$ and $\boldsymbol{P}$ are the center-of-mass coordinate and momentum of two electrons, $\boldsymbol{r}$ and $\boldsymbol{p}$ denote the coordinate and the momentum of the relative motion, respectively, M and μ are the total band mass and the reduced mass of two electrons, respectively, $e^2/(\varepsilon_\infty r)$ is the Coulomb potential between electrons, $m\Omega^2r^2/2$ is the confinement potential of the parabolic QD, in which Ω is the confinement potential strength, and a_k^+ and a_k are the creation and annihilation operators of a bulk OL phonon with wave vector $\boldsymbol{k}$, respectively. Assuming that the phonon frequency is not dispersive, $\omega_k=\omega_{\mathrm{LO}}$, then the interaction coefficient is written as

$$v_k=\frac{\square\hbar\omega_{\mathrm{LO}}}{k}\left[\frac{4\pi\alpha}{V}\left(\frac{\hbar\square}{2m\omega_{\mathrm{LO}}}\right)^{1/2}\right]^{1/2}\quad,\qquad(2)$$

where V is the volume of crystal and α is the dimensionless strength of the electron-phonon coupling written as

$$\alpha=\frac{e^2u_1}{2\hbar\omega_{\mathrm{LO}}}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right)=\frac{e^2}{2r_{\mathrm{p}}\hbar\omega_{\mathrm{LO}}}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right)\quad,\qquad(3)$$

where $\varepsilon_\infty(\varepsilon_0)$ is the high-frequency (static) dielectric constant and $r_{\mathrm{p}}=u_1^{-1}=\sqrt{\hbar/(2m\omega_{\mathrm{LO}})}$ is called the radius of a single polaron.

First, the Tokuda modified linear-combination operator is introduced into the center-of-mass coordinate and momentum of the bipolaron [14]

$$P_j=\left(\frac{M\hbar\lambda}{2}\right)^{1/2}\left(b_j^++b_j+p_{0j}\right),\ R_j=\mathrm{i}\left(\frac{\hbar}{2M\lambda}\right)^{1/2}\left(b_j-b_j^+\right)\ ,\ (4)$$

where λ and $\boldsymbol{p}_0$ are the variational parameters and $j=x, y, z$. To calculate the effective mass of the bipolaron, we discuss the extreme value problem of the expectation value of the operator function $J=U_2^{-1}U_1^{-1}(H-\boldsymbol{u}\cdot\boldsymbol{P}_{\mathrm{T}})U_1U_2$ in the state $|\Phi\rangle$.

$$\bar{J}=\left\langle\psi\left|U_2^{-1}U_1^{-1}(H-\boldsymbol{u}\cdot\boldsymbol{P}_{\mathrm{T}})U_1U_2\right|\psi\right\rangle\quad,\qquad(5)$$

where

$$\boldsymbol{P}_{\mathrm{T}}=\boldsymbol{P}+\sum_q\hbar\boldsymbol{k}a_k^+a_k\qquad(6)$$

is the total momentum of the system, and $\boldsymbol{u}$ is the Lagrange multiplier and will be identified as the center-of-mass velocity of the polaron.

$$U_1=\exp\left(-\mathrm{i}\sum_k\boldsymbol{k}\cdot\boldsymbol{r}a_k^+a_k\right),U_2=\exp\left(\sum_q\left(f_ka_k^+-f_k^*a_k\right)\right)\qquad(7)$$

is the Lee-Low-Pines unitary transformation [15], in which f_k and f_k^* are the variational parameters.

$$|\psi\rangle=\left|\{n_k\}\right\rangle\left|\{n_j\}\right\rangle\qquad(8)$$

is the trial wave function of the system under the finite temperature, in which $|n_k\rangle$ is the phonon state and $|n_j\rangle$ is the polaron state, $a_k|n_k\rangle=\sqrt{n_k}\,|n_k-1\rangle$, $a_k^+|n_k\rangle=\sqrt{n_k+1}\,|n_k+1\rangle$, $b_j|n_j\rangle=\sqrt{n_j}\,|n_j-1\rangle$, $b_j^+|n_j\rangle=\sqrt{n_j+1}\,|n_j+1\rangle$. According to the quantum statistics, the number of electrons n and the number of phonons n_k can be approximately replaced by the mean number

$$\bar{n}=\left[\exp\left(\frac{\hbar\lambda}{k_{\mathrm{B}}T}\right)+1\right]^{-1},\ \bar{n}_k=\left[\exp\left(\frac{\hbar\omega_{\mathrm{LO}}}{k_{\mathrm{B}}T}\right)-1\right]^{-1},\qquad(9)$$

where $\bar{n}=\bar{n}_j(j=x, y, z)$ when the symmetry of the electronic motion is considered, k_{B} is the Boltzmann constant, T is the thermodynamic temperature, and $\hbar\omega_{\mathrm{LO}}/k_{\mathrm{B}}T=\gamma$ is set as the temperature parameter.

Substituting Eqs.(1)-(4) and Eqs.(6)-(9) into Eq.(5), we can obtain

$$\bar{J}(f_k,f_k^*,\lambda,\boldsymbol{p}_0)=\frac{\boldsymbol{p}^2}{2\mu}+\frac{1}{2}\mu\,\Omega^2r^2+\frac{e^2}{\varepsilon_\infty r}+$$
$$\frac{3}{4}\hbar\left(\frac{\Omega^2}{\lambda}+\lambda\right)(2\bar{n}+1)+\frac{\hbar\lambda}{4}\boldsymbol{p}_0^2+\frac{\hbar^2}{2M}\sum_k\boldsymbol{k}^2\bar{n}_k+$$
$$\sum_k\bar{n}_k\hbar\omega_{\mathrm{LO}}\left(\bar{n}_k+|f_k|^2\right)-\left(\frac{M\hbar\lambda}{2}\right)^{1/2}\boldsymbol{u}\cdot\boldsymbol{p}_0+$$
$$\frac{\hbar^2}{2M}\sum_k\boldsymbol{k}^2|f_k|^2(4\bar{n}_k+1)-\frac{\hbar}{M}\left(\frac{M\hbar\lambda}{2}\right)^{1/2}\times$$
$$\sum_k\sum_jk_jp_{0j}\left(\bar{n}_k+|f_k|^2\right)+\frac{\hbar^2}{2\mu}\sum_k(\nabla f_k)(\nabla f_k^*)(2\bar{n}_k+1)+$$
$$2\sum_k\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{r}}{2}\right)\left(v_kf_k+\mathrm{H.c}\right).\qquad(10)$$

And then we calculate the extreme value $\bar{J}(f_k, f_k^*, \lambda, \boldsymbol{p}_0)$ to variational parameters. According to variational principle

$$\delta\bar{J}(f_k,f_k^*,\lambda,\boldsymbol{p}_0)=\delta\left[\left\langle\psi\left|U_2^{-1}U_1^{-1}(H-\boldsymbol{u}\cdot\boldsymbol{P}_{\mathrm{T}})U_1U_2\right|\psi\right\rangle\right]=0\ ,(11)$$

the variational parameters λ, f_k, f_k^* and $\boldsymbol{p}_0$ can be derived. The mean number of LO phonons $\bar{N}_{\mathrm{t}}$ is determined by using these variational parameters as

$$\bar{N}_{\mathrm{t}}=\left\langle\psi\left|U_1^{-1}U_2^{-1}\sum_qa_k^+a_kU_1U_2\right|\psi\right\rangle=\sum_k\bar{n}_k+\bar{N}\quad,\qquad(12)$$

where

$$\bar{N} = \sum_k \frac{4\cos^2\left(\frac{\boldsymbol{k}\cdot\boldsymbol{r}}{2}\right)|v_k|^2}{\left\{\frac{\hbar^2}{2M}\left[\boldsymbol{k}^2(4\bar{n}_k+1)+u_1^2\right]-\frac{\hbar}{M}\left(\frac{M\hbar\lambda}{2}\right)^{1/2}\boldsymbol{k}\cdot\boldsymbol{p}_0\right\}^2} \quad (13)$$

is the mean number of LO phonons of the bipolaron. Furthermore, based on these parameters, the average value of the total momentum can be given as

$$\boldsymbol{P}_{\mathrm{T}} = \langle\{n_k\}|\langle\{n_j\}|U_2^{-1}U_1^{-1}\boldsymbol{p}_{\mathrm{T}}U_1U_2|\{n_j\}\rangle|\{n_k\}\rangle = M^*\boldsymbol{u} \ , \quad (14)$$

where

$$M^* = M/\left\{1-\frac{16M^2}{\hbar^4}\sum_k \frac{\boldsymbol{k}^2|v_k^2|\cos^2\alpha}{\left[\boldsymbol{k}^2(4\bar{n}_k+1)+u_1^2\right]^3}\left[4\lambda\cos^2\left(\frac{\boldsymbol{k}\cdot\boldsymbol{r}}{2}\right)+\frac{3M\boldsymbol{k}^2\sin^2\left(\frac{\boldsymbol{k}\cdot\boldsymbol{r}}{2}\right)}{\mu\boldsymbol{k}^2(4\bar{n}_k+1)+u_1^2}(2\bar{n}_k+1)\right]\right\} \quad (15)$$

denotes the effective mass of the bipolaron in the QD. The contribution of the minor terms induced by the multi-phonon interaction and the higher-order minor terms of the wave vector can be ignored in the above derivation.

From Eq.(13) and Eq.(15), it can be found that the mean number $\bar{N}$ of LO phonons and the effective mass M^* of the bipolaron in the QD are related to the relative distance r between two electrons (called as electronic distance for short), the electron-LO phonon coupling strength α and the temperature parameter γ. Numerical results are shown in Fig.1−Fig.3 to describe the relation of $\bar{N}$ and M^* with r, α and γ, taking the total band mass M as the unit of mass, the polaronic radius r_{p} as the unit of length.

From Fig.1, it can be seen that $\bar{N}$ increases with increasing γ, in other words, $\bar{N}$ decreases with increasing T. Therefore, the mechanism of the electron-LO phonon interaction of the bipolaron in the QD is mainly the process that the electron firstly absorbs the phonon and then emits it. The thermal motion of the phonon around the electron is enhanced due to the increase of the temperature, so the interaction between the electron and the phonon around it is weakened, furthermore the mean number of phonons of the bipolaron decreasing. It is not hard to see that $\bar{N}$ increases rapidly with increasing γ when the value of γ is smaller (γ<5.22), but the variation of $\bar{N}$ with γ is not obvious when the value of γ is larger (γ>5.22). In addition, $\bar{N}$ increases with decreasing r, which shows that the medium around two electrons is polarized more strongly when two polarons are closer to each other, that is, the mean number of phonons around the bipolaron

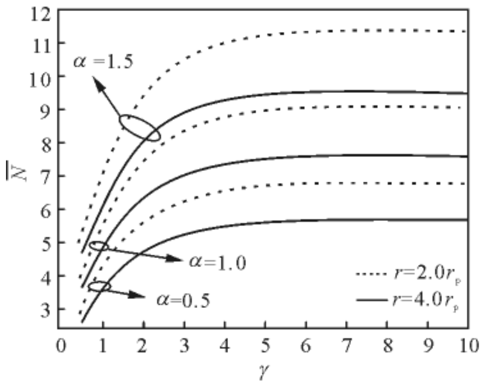

Fig.1 Relation between $\bar{N}$ and γ at various coupling strength α and relative distance r

increases. This result is consistent with the conclusion in Ref.[8]. According to Ref.[8], the induced potential $V_{\mathrm{e\text{-}LO}}$ caused by the electron-phonon coupling in the bipolaron is negative, and its absolute value $|V_{\mathrm{e\text{-}LO}}|$ increases with decreasing r. This shows that the interaction between two polarons caused by the electron-LO phonon coupling in the bipolaron is attraction, and this interaction will be stronger when two polarons are close to each other because the phonon number around two electrons increases. Moreover, we can see from Fig.1 that $\bar{N}$ also increases with increasing α. This is because the larger α means the stronger electron-phonon interaction, thus the polarization of the medium around electrons is enhanced, leading to the increase of the phonon number around electrons.

Fig.2 shows the variation of the effective mass of the bipolaron with the electronic distance r at various electron-phonon coupling strength α. It can be seen from Fig.2 that M^* increases rapidly with increasing r when the value of r is smaller (r<4.0r_{p}), and reaches a maximum at $r\approx 4.05r_{\mathrm{p}}$, and then M^* decreases slowly with increasing r. This shows that there is a fluctuating process in the variation of the density of phononic cloud of the bipolaron with r. The density of phononic cloud of the bipolaron increases with increasing r when r<4.05r_{p}, and reaches a maximum at $r\approx 4.05r_{\mathrm{p}}$, and then decreases slowly with the increase of r. From Fig.2, it can be also seen that M^* increases with increasing α. It is obvious because the larger α means the stronger electron-phonon interaction, and thus the polarization of the medium around two electrons is enhanced, which leads to the increase of the phonon number around electrons, further causing the increase of the effective mass of the bipoalron. In addition, the electron-phonon coupling strength α has remarkable influence on the variation of M^* with r. That is mainly shown by the fact that the slopes of M^*−r curves obviously increase with increasing α when r<4.05r_{p}; meanwhile, the extreme points of M^*−r curves go up obviously with increasing α.

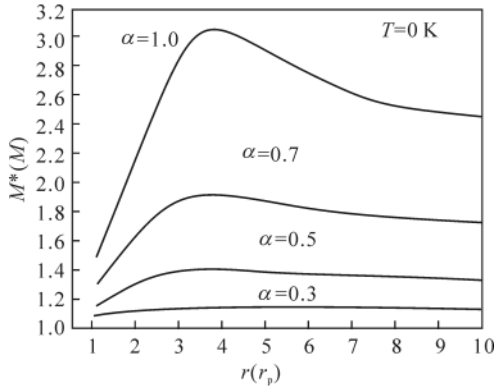

Fig.2 Relation between *M and *r* at various coupling strength α**

Fig.3 shows the variation of the effective mass M^* of the bipolaron with the temperature parameter γ at different electron-phonon coupling strengths. It can be seen that M^* increases with increasing γ, that is, M^* decreases with increasing T. Therefore, the mechanism of the electron-LO phonon interaction of the bipolaron in the QD is mainly the process that the electron firstly absorbs the phonon and then emits it. The thermal motion of the phonon around the electron is enhanced due to the increase of the temperature, thus the interaction between the electron and the phonon around it is weakened, further decreasing the mean number of phonons of the bipolaron, so the effective mass of the bipolaron decreases. From Fig.3, it can be also seen that the electron-phonon coupling strength α has remarkable influence on the variation of M^* with γ. This is mainly shown by the fact that the slopes of M^*−γ curves obviously increase with increasing α when γ<5.22 , while M^* increases slowly with increasing γ when γ>5.22. Furthermore, we can see $M_0^* \rightarrow M$ from Fig.3, where M_0^* is the starting point of M^*−γ curve, when $\gamma \rightarrow 0$ ($T \rightarrow \infty$) is satisfied, that is, the value of the effective mass of the bipolaron tends to the total band mass of two electrons. The physical meaning is that the electron loses its phonon cloud, and then turns to the quasi free electron because the thermal motion of the phonon around the electron is enhanced under the limiting condition of high temperature, namely the bipolaron is disintegrated.

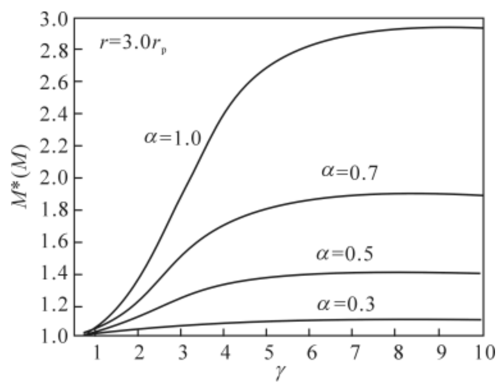

Fig.3 Relation between *M and γ at various coupling strength α**

In conclusion, the effects of the temperature and LO phonon on the effective mass of the biplaron in polar semiconductor QDs are studied by using the Tokuta modified linear-conbination operator method and the Lee-Low-Pines variational method. Numerical results show: The mean number of LO phonons $\bar{N}$ of the bipolaron decreases with increasing the temperature T and the relative distance r between two electrons, but increases with increasing the electron-phonon coupling strength α; The effective mass of the bipolaron M^* increases rapidly with increasing the relative distance r between two electrons when r is smaller, and it reaches a maximum at $r \approx 4.05r_p$, while after that, M^* decreases slowly with increasing r; The effective mass of the bipolaron M^* decreases with increasing the temperature; The electron-phonon coupling strength α markedly influences the changes of mean number of LO phonons $\bar{N}$ and the effective mass M^* with the relative distance r and the temperature parameter γ.

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