Effect of Temperature on the Energy of Polaron in a Parabolic Quantum Well

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【Abstract】 The influence of temperature on the ground state energy and ground state binding energy of polaron in a parabolic quantum well is studied by using the linear combination operator and unitary transformation methods. The expressions of the ground state energy and ground state binding energy of polaron are obtained by theoretical derivation. Combined with the expression of mean number phonons in quantum statistical mechanics, the function relationship between the ground state energy and ground state binding energy of polaron and temperature is obtained. When the temperature takes different values, the relationship between the ground state energy and the ground state binding energy with the electron-phonon coupling strength and well width is discussed respectively. The dependence of ground state energy and ground state binding energy on temperature is discussed when the well depth is taken at different values. The calculation results show that both the ground state energy and the ground state binding energy of the polaron are increasing functions of temperature.

Keywords: Parabolic quantum well, Ground state energy, Ground state binding energy, Temperature

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温度对抛物量子阱中极化子能量的影响

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【摘要】 采用线性组合算符法和幺正变换法研究温度对抛物型量子阱中极化子基态能和基态结合能的影响.通过理论推导得到极化子基态能和基态结合能的表达式.结合量子统计力学中平均声子数的表达式,得到极化子基态能量和基态结合能与温度的函数关系.在不同温度下,分别讨论了极化子基态能量和基态结合能与电子-声子耦合强度和阱宽的关系,阱深取不同值时讨论了极化子基态能和基态结合能随温度的变化规律.计算结果表明,极化子的基态能量和基态结合能都是温度的递增函数.

关键词: 抛物量子阱,基态能量,基态结合能,温度

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1 Introduction

With the in-depth study of semiconductor materials, many artificially designed quantum wells have been manufactured by molecular beam epitaxy and metal-organic chemical vapor deposition methods. And many interesting physical phenomena have been found in quantum well structures, which have important value for the research and development of new semiconductor devices. Quantum well devices are widely used in people's daily life. In recent years, the research on the properties of semiconductor quantum wells has become a research hotspot of low-dimensional semiconductor materials. Using a variety of methods, scholars have made experimental and theoretical research on the physical properties of quantum well structures[1-3]. For instance, Wei *et al.*[4] investigated the vibration magnetic field of the Coulomb impurity bound magnetopolaron in the GaAs/$Ga_{1-x}Al_xAs$ quantum well within MacDonald method. The bound magnetic polarons in dilute magnetic semiconductors were investigated by Wolf *et al.*[5] experimentally. Shan *et al.*[6] studied the effect of electric field on the properties of strong coupling magnetopolaron in triangular quantum wells. Under different electric fields, the relationship between the ground state binding energy of the polaron and the electron phonon coupling strength, magnetic field cyclotron frequency and electron surface density is obtained by numerical calculation. Wang *et al.*[7] studied the epitaxial growth of large mismatch InGaAs multi-quantum well on GaAs substrates using the same method. Due to the existence of the confinement potential, the properties of the polaron in the quantum well are significantly different from those of the electron. Since the 1990s, some researchers have also done a lot of research on the properties of parabolic quantum wells, and have made many research achievements. Parabolic quantum wells can be divided into two types, one is component parabolic quantum wells, and the other is doped parabolic quantum wells[8]. In recent years, scholars have studied the properties of two kinds of parabolic quantum well. Such as Zhang *et al.*[9] used the viriational method to calculate the binding energy of excitons of different Mn components in $Cd_{1-x}Mn_xTe$/CdTe parabolic quantum well under the effective mass approximation. The calculation results can provide a theoretical basis for the design and manufacture of semiconductor parabolic quantum well light-emitting devices. Shan[10] investigated the Rashba effect of the polaron in the RbCl parabolic quantum well, and obtained the expression of polaron ground state energy through theoretical derivation. Because of the Rashba spin orbit interaction, the ground state energy of the polaron is split into two branches. Sa *et al.*[11] studied the hydrogen-like impurity energy levels in infinite parabolic quantum well by using the variational method, and gave the functional relationship of energy with the well width and magnetic field strength under different magnetic fields. It can be seen that there have been a lot of researches on the properties of polarons in quantum wells, but so far, few people have studied the temperature effect of polarons in quantum wells. Ping *et al.*[12] used metal-organic chemical vapor deposition to grow three InGa/GaN quantum wells with different barrier temperatures, and analyzed the confinement Stark effect and carrier localization effect of quantum wells at different barrier temperatures. In this paper, the influence of temperature on the ground state energy and ground state binding energy of polaron in a parabolic quantum well is studied by using the unitary transformation and linear combination operator methods. When the temperature takes different values, the relationship among the ground state energy and ground state binding energy with the temperature is discussed, respectively. At the same time, the dependence of ground state energy and ground state binding energy on temperature is discussed when the well depth is taken at different values.

2 Theoretical derivation

The quantum well grows along the z direction, and the electron interacts with the bulk longitudinal optical phonon field, then the Hamiltonian of the electron-phonon system in the parabolic quantum well is

$$H=\frac{p_{//}^2}{2m}+\frac{p_z^2}{2m}+V(z)+\sum_q \hbar\omega_{LO}a_{\vec{q}}^+a_{\vec{q}}+\sum_q\left[V_q a_{\vec{q}}\exp(i\vec{q}\cdot\vec{r})+h.c.\right]. \quad (1)$$

Where m is the effective band mass of the electron, $V(z)$ is the parabolic potential energy, $a_{\vec{q}}^+(a_{\vec{q}})$ is the creation (annihilation) operator of the bulk longitudinal optical phonon with the wave vector $\vec{q}$ and frequency ω_{LO}, $\vec{r}=(\vec{\rho},z)$ is the position vector of the electron, and

$$V(z)=\begin{cases}V_0\left(\frac{z}{d}\right)^2, & |z|\leqslant d\\ V_0 & ,|z|>d\end{cases}, \quad (2)$$

$$V_q=i\left(\frac{\hbar\omega_{LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{LO}}\right)^{\frac{1}{4}}\left(\frac{4\pi\alpha}{V}\right)^{\frac{1}{2}}. \quad (3)$$

In Equations (2) and (3), V_0 is the parabolic potential well depth with the width well d, V_0 is the semiconductor volume, and V is the electron-phonon coupling strength.

Introducing the linear combination operator

$$p_j=\left(\frac{m\hbar\lambda}{2}\right)^{\frac{1}{2}}(b_j+b_j^+), \quad (4a)$$

$$r_j=i\left(\frac{\hbar}{2m\lambda}\right)^{\frac{1}{2}}(b_j-b_j^+). \quad (4b)$$

In Equation (4), $j=x,y,\lambda$ is variational parameter. Take the unitary transformation operator as

$$U=\exp\sum_q\left[f_q a_{\vec{q}}^+-f_q^* a_{\vec{q}}\right], \quad (5)$$

where f_q and f_q^* are variational parameters. The unitary transformed Hamiltonian is

$$H'=\frac{\hbar\lambda}{4}\sum_j(b_j^+b_j^++b_jb_j)+\frac{\hbar\lambda}{2}\sum_j(b_j^+b_j+1)+\frac{p_z^2}{2m}+\sum_q\hbar\omega_{LO}(a_{\vec{q}}^++f_q^*)(a_{\vec{q}}+f_q)+V_0\left(\frac{z}{d}\right)^2+\sum_q\{V_q(a_{\vec{q}}+f_q)\exp\left(-\frac{\hbar q^2}{4m\lambda}\right)\cdot\exp\left[-\left(\frac{\hbar}{2m\lambda}\right)^{\frac{1}{2}}\sum_j b_j^+q_j\right]\cdot\exp\left[\left(\frac{\hbar}{2m\lambda}\right)^{\frac{1}{2}}\sum_j b_jq_j\right]+h.c.\} \quad (6)$$

The ground state trial wave function of the system is selected as

$$|\Psi_0\rangle=|\varphi_z\rangle\,|0\rangle_a\,|0\rangle_b, \quad (7a)$$

$$\varphi_z=\left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}}\exp(-\beta z^2). \quad (7b)$$

Where $|0\rangle_a$ represents the perturbed zero phonon state and $|0\rangle_b$ is the vacuum state of the operator, which satisfies $b_j|0\rangle_b=a_{\vec{q}}|0\rangle_a=0$. We calculate

$$F(\lambda,f_q)=\langle\psi_0\,|\,H'\,|\,\psi_0\rangle=\frac{\hbar\lambda}{2}+\frac{p_z^2}{2m}+V_0\left(\frac{z}{d}\right)^2+\sum_q\hbar\omega_{LO}|f_q|^2+\sum_q(V_qf_q+V_q^*f_q^*)\exp\left(-\frac{\hbar q^2}{4m\lambda}\right). \quad (8)$$

Performing $\frac{\partial F}{\partial f_q}=0$ and $\frac{\partial F}{\partial f_q^*}=0$, we get

$$f_q^*=-\frac{\left[V_q\exp\left(-\frac{\hbar}{4m\lambda}q^2\right)\right]}{\hbar\omega_{LO}}, \quad (9a)$$

and

$$f_q=-\frac{\left[V_q^*\exp\left(-\frac{\hbar}{4m\lambda}q^2\right)\right]}{\hbar\omega_{LO}}. \quad (9b)$$

We substitute f_q and f_q^* into Equation (8), and replace the sum with an integral to get

$$F(\lambda,\beta')=\frac{\hbar\lambda}{2}+\frac{\hbar^2\beta'}{2m}+\frac{V_0}{4\beta'd^2}-\frac{\hbar\alpha\sqrt{\pi\lambda}}{2}\sqrt{\omega_{LO}}. \quad (10)$$

Performing the variation of $F(\lambda)$ with respect to λ, we obtain

$$\frac{\hbar}{2}-\frac{1}{4}\alpha\hbar\sqrt{\omega_{LO}\pi}\lambda^{-\frac{1}{2}}=0. \quad (11)$$

By solving equation (11), we get the vibrational frequency λ_0 of the polaron.

By substituting λ_0 into Eq. (10), we obtain the polaron ground state energy E_0.

$$E_0 = \frac{\hbar\lambda}{2} + \frac{\hbar^2\beta'}{2m} + \frac{V_0}{4\beta' d^2} - \frac{\hbar\alpha\sqrt{\pi\lambda\omega_{LO}}}{2}. \quad (12)$$

If E_e and E_p denote the energies of the uncoupled electron and phonon, respectively, then the ground state binding energy of the polaron is given by

$$E_b = E_e + E_p - E_0 = \hbar\alpha\sqrt{\pi\lambda\omega_{LO}} - \frac{V_0}{4\beta' d^2}. \quad (13)$$

Where

$$E_e = \frac{\hbar\lambda}{2} + \frac{\hbar^2\beta'}{2m}, \quad (14)$$

and

$$E_p = \frac{\hbar\alpha\sqrt{\pi\lambda}}{2}\omega_{LO}. \quad (15)$$

We solve the mean number phonons, which can be expressed as

$$\overline{N} = \langle \psi_0 \mid U^{-1}\sum_q a_{\vec{q}}^{+} a_{\vec{q}} U \mid \psi_0 \rangle = \frac{\alpha}{2}\sqrt{\frac{\pi\lambda}{\omega_{LO}}}. \quad (16)$$

At a finite temperature, the electron-phonon system will no longer be complete in the ground state. The lattice vibration not only excites the real phonon, but also excites the electron. The properties of the polaron are determined by the statistical average of the various states of the electron-phonon system. In quantum statistics, the expression of the mean number of phonon is

$$\overline{N} = \left[\exp\left(\frac{\hbar\omega_{LO}}{K_B T}\right) - 1\right]^{-1}. \quad (17)$$

Where K_B is the Boltzmann constant, and the value is 1.38×10^{-23} J/K. Obviously, the value of λ in Eq. (16) is related to $\overline{N}$. Combining Eq. (16) and (17), we can get the relationship between E_0, E_b and T.

3 Numerical calculation and result discussion

From the expressions of the ground state energy and ground state binding energy of the polaron, it can be seen that the ground state energy and ground state binding energy of the strong coupled polaron are not only related to the well width and well depth, but also to the electron-phonon coupling strength and vibration frequency. In order to more clearly show the influence of temperature on the ground state energy and ground state binding energy of polaron in a parabolic quantum well, we perform numerical calculations for the polaron ground state energy and ground state binding energy, respectively. The calculation results are shown in Fig. 1 to 6. To simplify the calculation, polaron units ($\hbar = 1, 2m = 1, \omega_{LO} = 1$) are taken.

Fig. 1 shows the relationship between the ground state energy E_0 of the strong coupled polaron and the electron-phonon coupling strength α in a parabolic quantum well when the temperature T takes different values. One can see from the figure that the ground state energy is a decreasing function of the electron-phonon coupling strength. When the electron phonon coupling strength for a fixed value, the higher the temperature is, the greater the polaron ground state energy is. With the increase of electron-phonon coupling strength, the electron-phonon interaction is enhanced, and more phonons interact with the electron. However, in Eq. (10), the electron-phonon coupling strength has a negative effect on the ground state energy. Therefore, with the increase of electron-phonon coupling strength, the ground state energy of the polaron increases. It is also

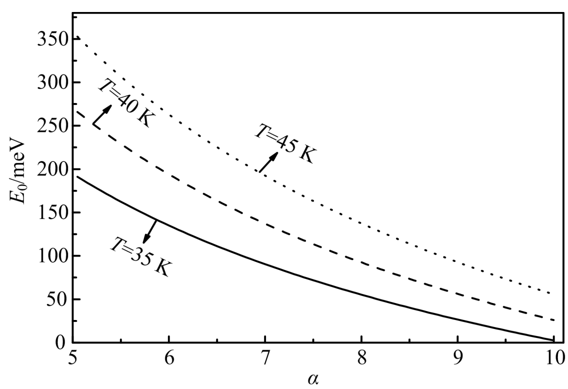

Fig. 1 The relationship between the ground state energy E_0 and electron-phonon coupling strength α at different values of temperature T.

found from the figure that the influence of temperature on ground state energy decreases with the increase of electron phonon coupling strength.

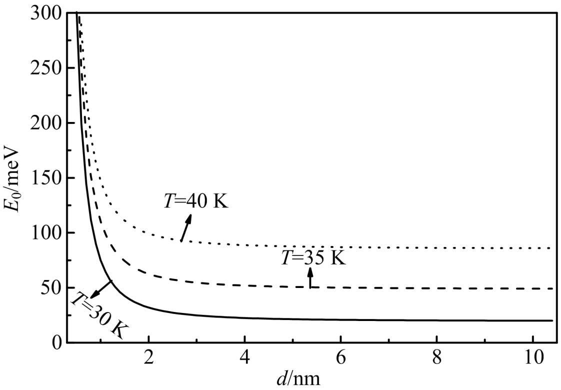

Fig. 2 The relationship between the ground state energy E_0 and well width d at different values of temperature T.

With different values of temperature T, Fig. 2 describes the relationship between the ground state energy E_0 of the polaron and the well width d. It can be seen from the figure that when the well width $d<1$ nm, the ground state energy increases rapidly as the well width decreases, and the temperature has little influence on the ground state energy. Beyond this range, with the increase of the well width, the ground state energy slowly decreases until it remains unchanged. This indicates that the quantum confinement effect is related to the well width, and the smaller the well width is, the more significant the quantum confinement effect is. When the well width is fixed, the higher the temperature is, the greater the ground state energy of the polaron is, which is consistent with the conclusion in Fig. 1. Under different well depths, Fig. 3 illustrates the functional relationship curve between ground state energy E_0 and temperature T. We find from the figure that the ground state energy is an increase function of the temperature. This conclusion is the same as the Fig. 1 and Fig. 2. We also find that the ground state energy of polaron increases with the increase of well depth. The electron phonon interaction is enhanced with the increase of the well depth, that is, the larger the well depth is, the greater the interaction energy is, resulting in the larger ground state energy of the polaron.

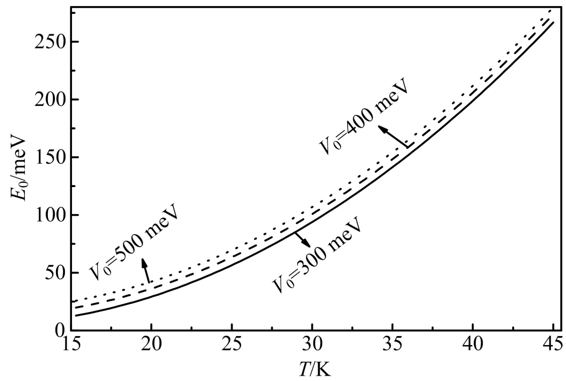

Fig. 3 The relationship between the ground state energy E_0 and temperature T at different values of well depth V_0.

Fig. 4 describes the relationship between the ground state binding energy E_b of the strong coupled polaron and the electron-phonon coupling strength α in the parabolic quantum well at different temperatures T. It can be seen from the figure that the ground state binding energy is an increase function of the temperature and electron-phonon coupling strength. It is also found that with the increase of the electron-phonon coupling strength, the influence of temperature on the ground state energy gradually increases. This conclusion is contrary to Fig. 1. For different values of temperature T, Fig. 5 shows the curve of the ground state binding energy E_b of polaron as a function of the well width d. As shown in the figure, when the well width $d<1$ nm, the ground state binding energy increases rapidly with the increase of the well width. Beyond this range, the ground state binding energy changes little with the increase of the well width, indicating that the electron phonon interaction is weak. In the figure, the ground state binding energy is an increasing function of temperature. In Eq. (13), the confined potential is inversely proportional to the square of the well width, that is, the confined potential decreases with the increase of the well width. In the expression of the ground state binding energy of the polaron, the influence of the confined potential on the ground state binding energy is negative. At the same time, with the increase of the well width, the electron phonon interaction weakens, that is, the ground state energy of the polaron decreases with the increase of well width, so the ground state binding energy of the polaron increases with the increase of the well width.

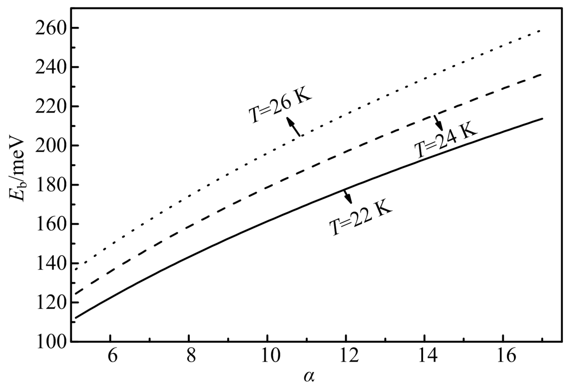

Fig. 4　The relationship between the ground state binding energy E_b and electron-phonon coupling strength α at different values of temperature T.

Fig. 6 draws the functional relationship curve between the ground state binding energy E_b of polaron and temperature T under different well depths V_0. It can be seen from the figure that the ground state binding energy of polaron is an increase function of temperature and a decreasing function of well depth. According to Eq. (13), the contribution of the well depth to the ground state binding energy is negative, so the binding energy decreases with the increase of the well depth. From Fig. 1 to Fig. 6, we find that both the ground state energy and the ground state binding energy of the polaron are increasing functions of temperature. Because the polarization of the crystal increases with the increase of temperature, the electron phonon interaction is enhanced. In other words, with the increase of temperature, there are more phonons interacting with electrons in the electron cloud around the electron.

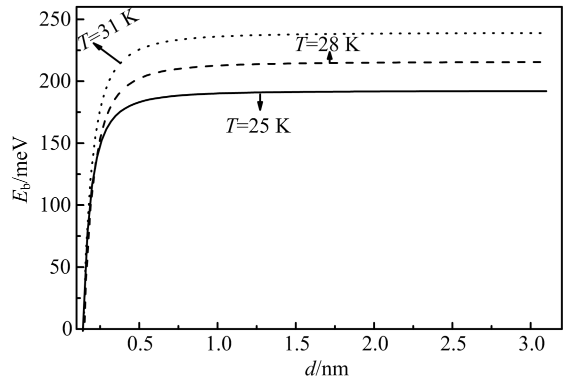

Fig. 5　The relationship between the ground state binding energy E_b and well width d at different values of temperature T.

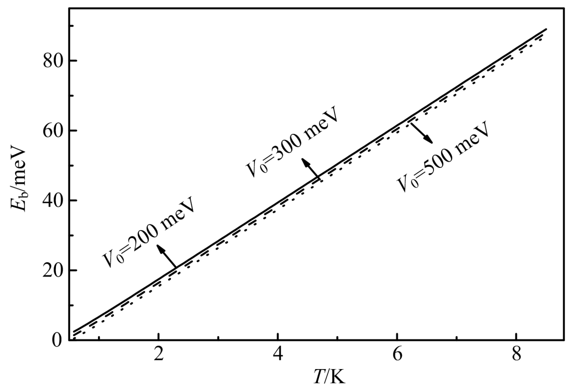

Fig. 6　The relationship between the ground state binding energy E_b and temperature T at different values of well depth V_0.

4　Conclusion

The expressions of the ground state energy and ground state binding energy of the polaron are obtained by using unitary transformation and linear combination operator methods. The expression of the mean number phonons of polaron is derived theoretically. The polaron ground state energy, ground state binding energy, and mean number phonons are all functions of vibrational frequency. Combined with the expression of mean number phonons in quantum statistical mechanics, the function relationship between the ground state energy and ground state binding energy of polaron and temperature is obtained. When the temperature takes different values, the

relationship between the ground state energy and the ground state binding energy with the electron-phonon coupling strength and well width is discussed respectively. The dependence of ground state energy and ground state binding energy on temperature is discussed when the well depth is taken at different values. The calculation results show that both the ground state energy and the ground state binding energy of the polaron are increasing functions of temperature.

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