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Influence of temperature and spin-orbit interaction on the effective mass of polaron in an anisotropic quantum dot

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Abstract: Using Tokuda's improved linear combination operator method and variational technique, the expression of the effective mass of strong coupled polaron in an anisotropic quantum dot is derived. Due to the spin orbit interaction, the effective mass of polaron splits into two branches. The dependence of effective mass on temperature, electron-phonon coupling strength, transverse and longitudinal confinement lengths and velocity is discussed by numerical calculation. The effective mass of polaron is an increasing function of temperature and electron-phonon coupling strength, and a decreasing function of transverse confinement length, longitudinal confinement length, and velocity. The absolute value of spin splitting effective mass increases with the increase of temperature and spin orbit coupling parameter, and decreases with the increase of transverse confinement length, longitudinal confinement length and velocity. Due to the heavy hole characteristic, the spin splitting effective mass is negative.

Key words: Anisotropic quantum dot, Effective mass, Heavy hole characteristic, Rashba effect

0 Instruction

A fundamental problem in spintronics is the injection of spin-polarized electrons into semiconductors to make devices. How to control and manipulate electron spin in semiconductor materials is a hot topic in material device research[1,2]. By utilizing electronic spin, electronic devices with new physical properties can be manufactured, such as magnetic random access memories, spin field-effect transistors, spin controlled lasers, etc. These devices rely on the ability to control the spin of electrons in solids, aiming to reduce power consumption, overcome the speed limit associated with electronic charges, and be used for quantum information processing and quantum computing in the future[3,4,5]. In recent years, spintronics has become one of the most popular research fields in physics. Researchers have done extensive research on spintronics and achieved rich research results[6,7]. Semiconductors are the best material for studying spintronics. First, they have fewer carriers, allowing the study of single electron behaviour, without the multi-body effect. Secondly, semiconductor single crystals or heterostructures, quantum wells, superlattice, and quantum dots can be made in very good quality, so that lattice defects and impurities can be minimized, and electronic spin relaxation can be reduced. [8]The spin properties of an electron in a semiconductor are not only determined by its own magnetic moment, but more importantly are related to its orbital motion. The Rashba splitting caused by spin-orbit coupling is more pronounced in narrow bandgap semiconductors. The Rashba effect plays an important role in semiconductor spintronics, which has attracted many scholars' attention in recent years. For example, considering the external magnetic field, Babayev et al.[9] theory studied the influence of Rashba effect on the properties
of a semiconductor quantum-antiwire and calculated the Rashba spin orbit splitting energy. Lipparini et al.[10] studied the spin-orbit effect in GaAs quantum wells, with a focus on the interaction between the Rashba effect, Dresselhaus effect, and Zeeman effect. Electron spin has also been experimentally studied, such as Qiu and Gui et al.[11], who studied the giant Rashba effect in HgTe quantum wells with inverted energy bands. The spin orbit splitting of III-V semiconductors is a linear term of momentum in the Hamiltonian of the system, which results in the dispersion relation of electron energy, and the energy is split from one parabola into two. However, in the HgTe quantum well, the electrons have the characteristics of heavy holes, the band gap is negative, and the conduction band and the valence band have Strong interaction, so the conduction band and the valence band have serious nonparabolism, resulting in a huge Rashba spin orbit splitting of energy, and the experiment shows that the electron spin orbit splitting energy appears k. However, the electron has heavy hole characteristics in the HgTe quantum well, and the bandgap width is negative. The conduction band and valence band have a strong interaction, so the conduction band and valence band have serious nonparabolicity, resulting in huge Rashba spin orbit splitting energy. The experiment results show that the electron spin orbit splitting energy appears \( k^3 \).

The Rashba effect of polaron with heavy hole characteristics in an asymmetric quantum dot was investigated within the Pekar variational method by the author of this article, and the conclusion obtained is consistent with the experiment. On the basis of previous research, this article uses Tokuta's improved linear combination operator method to continue studying the impact of the Rashba effect on the effective mass of polaron with heavy hole characteristics in an anisotropic quantum dot. No one has ever conducted research on this issue before.

2 Theoretical model and derivation

Selecting an anisotropic quantum dot structure, the motion of electron with heavy hole characteristic is strongly restricted in three dimensions. We only consider the interaction between the electron and longitudinal optical phonons, and ignore the interaction between the electron and interface optical phonons. The Hamiltonian of the system can be written as[12]

\[
H = \frac{\mathbf{P}^2}{2m} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k},o} a^\dagger \mathbf{c} a + \frac{1}{2} m \omega^2 \rho^2 + \frac{1}{2} m \omega^2 z^2 + \sum_{\mathbf{k}} [V_{\mathbf{k}} a^\dagger a \exp(i \mathbf{k} \cdot \mathbf{r}) + h.c.] \\
+ i \frac{\alpha_{\mathbf{k}}}{2 \hbar} \left( \hat{\mathbf{p}}^\dagger \hat{\sigma}_+ - \hat{\mathbf{p}}^\dagger \hat{\sigma}_- \right) 
\]  

In equation (1), The last term represents the Hamiltonian that only considers band splitting of heavy hole states in the spin orbit coupled effect. Where \( P_{\pm} = P_x \pm iP_y, \sigma_{\pm} = \sigma_x \pm i\sigma_y \).

In equation (1), \( V_{\mathbf{k}} \) is the Fourier component of electron phonon interaction, it can be expressed as
\[ V_k = i \left( \frac{\hbar \omega_{1,0}}{k} \right)^{1/4} \left( \frac{\hbar}{2m\omega_{1,0}} \right)^{1/4} \left( 4\pi \alpha \right)^{1/2}. \] (2)

The meanings of each physical quantity in equation (1) and (2) are the same as those in reference[12] will no longer be expressed. Due to the strong coupling studied, we perform the second unitary transformation on equation (1), and under the adiabatic approximation, take the unitary transformation operator as

\[ U = \exp \left[ \sum_k \left( a_k^* f_k - a_k f_k^* \right) \right]. \] (3)

Here \( f_k \) and \( f_k^* \) are variational parameter functions that can be obtained through variational techniques.

Introducing Tokuta’s improved linear combination operators

\[ p_j = \left[ \frac{m\hbar \lambda}{2} \right]^{1/2} (b_j + b_j^* + P_0), \] (4a)

\[ r_j = i \left[ \frac{\hbar}{2m\lambda} \right]^{1/2} (b_j - b_j^*), \] (4b)

\( j = x, y, z \). Here \( \lambda \) and \( P_0 \) are variational parameters, and \( \lambda \) represents the vibrational frequency of the polaron. The ground state trial wave function of the system is selected as:

\[ |\psi_0\rangle = (c \chi_{1/2} + d \chi_{-1/2}) \langle 0 |_{a,\downarrow} | 0 \rangle_{b,\uparrow}. \] (5)

The vacuum state \( |0\rangle_{b} \) of the \( b \) operator and the unperturbed zero phonon state \( |0\rangle_{a} \) satisfy \( b_j |0\rangle_{b} = a_k |0\rangle_{a} = 0 \). \( \chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \) and \( \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \) represent spin-up and spin-down states, respectively. In order to obtain the effective mass of strong coupled polaron, the minimum energy of the polaron can be obtained by controlling the total momentum of the system. The total momentum operator is written as

\[ P_T = P + \sum_k a_k^* a_k \hbar k. \] (6)

The ground state trial wave function \( |\psi_0\rangle \) acts on formula \( U^{-1}(H - u \cdot P_T)U \), and its expected value is

\[ F(\lambda, f_k, u, P_0) = \langle \psi_0 | U^{-1}(H - u \cdot P_T)U | \psi_0 \rangle. \] (7)

Equation (8) takes the variation for \( f_k \) and \( f_k^* \), takes the minimum value of the variation, and obtains \( f_k \) and \( f_k^* \), then take them into \( F \). We have
\[ F(\lambda, P_0, u) = \frac{3}{4} \hbar \lambda + \frac{1}{4} \hbar \lambda P_0^2 + \frac{\hbar \omega^2}{2 \lambda} + \frac{\hbar \omega^2}{4 \lambda} - u P_0 \left( \frac{m \hbar \lambda}{2} \right)^{\frac{3}{2}} - \frac{\alpha}{\sqrt{\pi}} h \sqrt{\lambda \omega_{LO}} - \alpha \frac{\hbar^2}{3 \sqrt{\pi}} \left( \frac{\lambda}{\omega_{LO}} \right)^{\frac{3}{2}} m u^2 \pm \frac{\alpha m \lambda}{\hbar^3} \left( \frac{m \hbar \lambda}{2} \right)^{\frac{3}{2}} (p_0 - p_0) \]  

(8)

We ignore the higher order term of \( p_0 \). Using variational method, \( p_0 \) is obtained, then take it into Equation (8). Then \( F \) takes the variation of \( \lambda \), and the expression of the vibration frequency of the polaron can be obtained by taking the extreme value. The vibration frequency \( \lambda \) satisfies

\[ \lambda^2 - \frac{\alpha u^2}{3 \sqrt{\pi}} \lambda^{\frac{3}{2}} - \frac{2}{3} \alpha \sqrt{\frac{\omega_{LO}}{\pi}} \lambda^{\frac{3}{2}} - \frac{1}{3} \left( \frac{8}{l_1^2} + \frac{4}{l_2^2} \right) = 0. \]  

(9)

Assuming that the root of the above equation is \( \lambda = \lambda_0 \), and let \( l_1 = \sqrt{\frac{h}{m \omega_1}} \), \( l_2 = \sqrt{\frac{h}{m \omega_2}} \). \( l_1 \) and \( l_2 \) are the transverse and longitudinal effective confinement lengths, respectively.

The expected value of momentum is

\[ p = \frac{1}{u} \left[ <\psi_0|U^{-1}HU|\psi_0> - F \right] = m \left[ 1 + \frac{2 \alpha}{3 \sqrt{\pi}} \left( \frac{\lambda}{\omega_{LO}} \right)^{\frac{3}{2}} \left( \pm \frac{\alpha m \lambda}{\hbar^2 u} \right) \right] u. \]  

(10)

In equation (10), \( u \) is defined as the velocity of the polaron, and the factor before \( u \) is

\[ m^* = m \left[ 1 + \frac{2 \alpha}{3 \sqrt{\pi}} \left( \frac{\lambda}{\omega_{LO}} \right)^{\frac{3}{2}} \left( \pm \frac{\alpha m \lambda}{\hbar^2 u} \right) \right], \]  

(11)

which represents the effective mass of polaron.

The mean number of phonons around the electron is:

\[ N = <\psi_0|U^{-1} \sum_k a_k^* a_k|\psi_0> = \frac{\alpha}{\sqrt{\pi}} \sqrt{\lambda_0}. \]  

(12)

The properties of polaron are determined by the statistical mean of the electron-phonon system for various states. According to the quantum statistics:

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

(13)

The value of \( \lambda \) in Equation (11) is related to \( \overline{N} \), and the relationship between \( m^* \)
and \( T \) can be obtained by combining equations (12) and (13).

3 Numerical calculation and result discussion

In order to investigate the temperature effect and the Rashba effect of the strong coupled polaron effective mass in an anisotropic quantum dot, the effective mass of the polaron is calculated numerically, and the changes of effective mass with temperature, transverse confinement length, longitudinal confinement length, electron-phonon coupling strength, and velocity are discussed. In order to simplify the calculation, polaron units \( 2m = 1, \hbar = 1 \) and \( \omega_{LO} = 1 \) are used. Because of the strong coupling, the electron-phonon coupling strength value will be taken \( \alpha \geq 6 \) during the calculation process. The numerical calculation conclusions are shown in Figs. 1 to 8. From figure 1 to figure 4, the solid line represents the zero spin effective mass \( m^*_0 \), the short solid line represents the spin-up splitting effective mass \( m^*_+ \), and the dotted line represents the spin-down splitting effective mass \( m^*_− \).

Fig.1 The relationship between the effective mass \( m^* \) of polaron and temperature \( T \) at different values of electron phonon coupling strength \( \alpha \).

With fixed values \( l_1 = 1, l_2 = 1.2, \alpha_R = 1.5 \) and \( u = 2 \), figure 1 shows the variation curve of the effective mass \( m^* \) of the polaron with temperature \( T \) when the electron-phonon coupling strength \( \alpha \) takes different values. When \( \alpha = 6, l_2 = 1.2, \)
\( \alpha_r = 1.5 \) and \( u = 2 \), figure 2 depicts the relationship between the effective mass \( m^* \) of the polaron and the temperature \( T \) with different values of the transverse confinement length \( l_1 \). Given \( \alpha = 6 \), \( l_1 = 0.8 \), \( \alpha_r = 1.5 \) and \( u = 2 \), figure 3 shows the curve of the polaron effective mass \( m^* \) with temperature \( T \) at different values of the longitudinal confinement length \( l_2 \). As can be seen from the three figures, the temperature is an increasing function of the polaron effective mass. Because the polarization degree of the crystal increases with the increase of the temperature, the electron phonon interaction increases. That is, as the temperature increases, more phonons interact with the electron, so that the effective mass of the polaron increases with the increase of the temperature. In the three figures, it is also found that the effective mass splits into two branches based on the zero spin. From the expression of effective mass, it can be seen that the spin-orbit interaction term has split. Due to the structure inversion asymmetry in the semiconductor heterojunction, the Rashba spin orbit splitting occurs at the Fermi surface. As can be seen in the above figures, when the temperature is low, the effective mass splitting is not significant. As the temperature increases, the splitting distance increases. This indicates that the temperature has a positive effect on the Rashba effect. In Figure 1, when the temperature is fixed, the larger the electron-phonon coupling strength is, the larger the effective mass of the polaron is. This is because as the electron-phonon coupling strength increases, the interaction between electron and its surrounding phonons increases, and more phonons interact with the electron, resulting in an increase in effective mass. It is also found that the effective mass splitting is significant when the electron-phonon coupling strength is small. Although there is no electron-phonon coupling strength in the effective mass splitting, it is related to the vibrational frequency. Therefore, the electron-phonon coupling strength is indirectly reflected in effective mass splitting and has an impact on splitting. In Figures 2 and 3, the smaller the transverse and longitudinal confinement lengths are, the greater the effective mass of the polaron is. As is known from formulas \( l_1 = \sqrt{\frac{\hbar}{m \omega_1}} \) and \( l_2 = \sqrt{\frac{\hbar}{m \omega_2}} \), the confinement length is inversely proportional to the square root of the confinement potential. The existence of the confinement potential limits the motion of the polaron. The larger the confinement potential is, the more obvious the quantum size effect is, that is, the smaller the confinement length is, the greater the effective mass of the polaron is. From the two figures, it also can be seen that the influence of the transverse confinement length on the effective mass is lager than that of the longitudinal confinement length.

With the fixed values \( \alpha = 6 \), \( l_1 = 1.0 \), \( l_2 = 1.2 \), \( \alpha_r = 1.5 \), figure 4 shows the
relationship curve between the effective mass $m^*$ of the polaron and the velocity $u$

![Graph showing the relationship between effective mass $m^*$ and temperature $T$ for different values of $l_1$.](image1)

Fig. 2 The relational curve between the effective mass $m^*$ and temperature $T$ when the transverse confinement length $l_1$ takes different values.

![Graph showing the relationship between effective mass $m^*$ and temperature $T$ for different values of $l_2$.](image2)

Fig. 3 The relational curve between the effective mass $m^*$ and temperature $T$ when the longitudinal confinement length $l_2$ takes different values.
Fig. 4 The relationship between the effective mass $m^*$ and the velocity $u$ of polaron at different temperature values when the temperature $T$ takes different values. As shown in the figure, when the temperature is fixed, the effective mass of the polaron splits into two curves based on zero spin splitting, and the two curves have opposite changing trends with increasing velocity. When the polaron velocity $u < 1$, the two curves change significantly with the increase of the polaron velocity, and the spin-up splitting effective mass decreases significantly with the increase of the polaron velocity, the spin-down splitting effective mass increases significantly with the increase of polaron velocity. Outside this region, the spin-up splitting effective mass and spin-down splitting effective mass of polaron changes slowly with the increase of the velocity, and the two curves tend towards zero spin effective mass, but do not coincide with the zero spin effective mass curve. This phenomenon indicates that the smaller the polaron velocity is, the more significant the effect on effective mass spin splitting is. From the expression of effective mass, it can also be seen that the velocity is inversely proportional to the spin splitting effective mass, so the conclusion in the figure will be obtained. It is also found that the zero spin effective mass curve is parallel to the horizontal axis, indicating that the velocity has no effect on the zero spin effective mass. When the velocity is determined, the higher the temperature is, the larger the effective mass is. This conclusion is consistent with that of Figs. 1, 2 and 3. When the velocity is small, as the velocity decrease, the distance between the spin-up splitting effective mass curves becomes smaller and smaller at different temperatures, and the distance between the spin-down splitting effective mass curves tends to overlap with the decrease of the velocity. It shows that the effect of temperature on the spin splitting effective mass is affected by the velocity. The smaller the velocity is, the smaller the
effect of temperature on the effective mass splitting is. When \( \alpha_R = 1.5, l_1 = 1.2, u = 2 \), and the transverse confinement length \( l_1 \) takes different values, Fig.5 shows the relationship between the spin splitting effective mass \( m_{SO}^* \) and temperature \( T \).

Figure 6 shows the relationship between the spin splitting effective mass \( m_{SO}^* \) and temperature \( T \) when \( \alpha_R = 1.5, l_1 = 1.2, u = 2 \), and the longitudinal confinement length \( l_2 \) takes different values. Given fixed values \( l_1 = 0.6, l_2 = 1.0 \) and \( u = 2 \), and different values for spin orbit coupling parameters, figure 7 shows the relationship curve between spin splitting effective mass \( m_{SO}^* \) and temperature \( T \). It is found from the three figures that the absolute value of the spin splitting effective mass increases with the increase of temperature, indicating that the contribution of temperature to the spin splitting effective mass is positive. Fig.5 and Fig.6 show that when the temperature is constant, the smaller the transverse or longitudinal confinement length is, the larger the absolute value of the spin splitting effective mass is. Moreover, as the temperature increases, several curves tend to approach each other, indicating that the influence of the confinement length on the spin splitting effective mass is weakened with the increase of temperature. Comparing Fig.5 and Fig.6, the influence of transverse confinement length on the spin splitting effective mass is greater than that of longitudinal confinement length. Figure 7 shows that when the temperature is fixed, the larger the spin orbit coupling parameter is, the larger the absolute value of the spin splitting effective mass is, and the influence of spin orbit coupling parameter on the spin splitting effective mass gradually increases with the increase of temperature. In the expression \( m_{SO}^* = -\frac{2\alpha_R m l^2}{\hbar^2 u} \) of the spin splitting effective mass, it is found that the spin orbit coupling parameter is proportional to the spin splitting effective mass, so the above conclusion is obtained. The temperature \( T \) takes different values, Fig.8 depicts the change curve of the spin splitting effective mass \( m_{SO}^* \) with the velocity \( u \) for fixed \( \alpha_R = 1.5, l_1 = 2, l_2 = 2.5 \). It is found that when the velocity is fixed, the absolute value of the spin splitting effective mass increases with the increase of temperature. When the velocity \( u < 0.5 \), the influence of temperature on the spin splitting effective mass gradually increases with the increase of the velocity. When \( u > 0.5 \), the influence of temperature on the spin splitting effective mass gradually decreases with the increase of the velocity. An interesting phenomenon is found in figures 5, 6, 7, and 8, where the spin splitting effective mass is negative, due to the heavy hole characteristics of the studied spin orbit splitting.
Fig. 5 The relational curve between the spin splitting effective mass $m_{so}^*$ and temperature $T$ at different values of the transverse confinement length $l_1$.

Fig. 6 The relational curve between the spin splitting effective mass $m_{so}^*$ and temperature $T$ at different values of the longitudinal confinement length $l_2$. 
Fig. 7 The variation curve of the spin splitting effective mass $m_{so}^*$ with temperature T when the spin-orbit coupling parameter $\alpha_R$ takes different values.

Fig. 8 The relationship between the spin splitting effective mass $m_{so}^*$ of polaron and the velocity $u$ at different temperatures

4 Conclusion

The temperature effect and the Rashba effect of the effective mass of strong coupled polaron in an anisotropic quantum dot is studied theoretically. Under the influence of
Rashba effect, the effective mass of the polaron splits into two branches on the basis of zero spin. With the increase of temperature, the effective mass increases, and the splitting distance of effective mass increases, indicating that the influence of temperature on the effective mass and the spin splitting effective mass is positive. We also studied the effects of transverse confinement length, longitudinal confinement length, and polaron velocity on the effective mass and spin splitting effective mass. The results show that the smaller the confinement length is, the larger the effective mass of the polaron is, which reflects the strange quantum limiting effect. With the increase of the polaron velocity, the spin-up and spin-down splits of effective mass change in reverse law, and the last two splits tend to the value of effective mass with zero spin splitting. We obtain an interesting conclusion that the spin splitting effective mass is negative. This is because spin orbit coupled splitting only takes into account the splitting of the heavy hole band, so the spin splitting effective mass is negative.

References