

The properties of the polaron in semiconductor quantum dots induced by influence of Rashba spin-orbit interaction

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Abstract. The properties of the effective mass of polaron in semiconductor quantum dots by influence of Rashba spin-orbit (SO) interaction are studied. The relations of the strength of confinement ω_0 , the interaction energy and the effective mass of the polaron in the electron-LO phonon strong coupling region in a parabolic quantum dot on the vibration frequency is derived by using improved linear combination operator method. Numerical calculations for RbCl crystal are performed and the results show that the Rashba SO interaction makes the ground state energy and the effective mass of polaron split into two branches; the ground splitting energy and the effective mass will increase with the vibration frequency increasing. Whereas the interaction energy is sharply increased until the confinement strength reaches a certain value, then it will sharply decrease.

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Key words: semiconductor quantum dot, polaron, Rashba spin-orbit interaction, effective mass

1 Introduction

In recent years there has attracted great attention in spin physics in semiconductors. Most of it is focused on spin-related optical and transport properties of low-dimensional semiconductor structures [1-3]. In particular, the spin-orbit (SO) interaction has attracted a lot of interest as it plays an important role in the field of semiconductor spintronics. SO interaction can arise in quantum dots (QDs) by various mechanisms related to electron confinement and symmetry breaking and are generally introduced in the Hamiltonian via the Rashba [4] and Dresselhaus terms [5]. Dresselhaus term is obtained from the electric field produced by the bulk inversion asymmetry of the material and Rashba term is

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generated due to the structural asymmetry of the heterostructure. Rashba splitting has been observed in many experiments and it constitutes the basis of the proposed electronic nanostructures. The strength of these interactions not only depends on the characteristics of the material but can be controlled by an external electric field.

In the literature, most of the theoretical studies about the solution of the SO effects in QDs are carried out by means of perturbative schemes or numerical simulations [6, 7]. Analytical solution of the problem has recently been treated by employing various techniques [8-11]. For zero-magnetic field and a hard-wall confining potential the exact analytical results have been obtained by Boulgakov and Sadreev[12]. Tsitsishvili et al present an analytic solution to Rashba coupling in a quantum dots [13]. Tapash Chakraborty report on a theoretical approach developed to investigate the influence of the Bychkov-Rashba interaction on a few interacting electrons confined in a quantum dot [14].

There have been much work about the influence of the Rashba SO interaction on the electron system, the study of the effect of the Rashba SO interaction on the polaron, however, is quite rare so far. In this paper, we find the Rashba SO will induce the splitting of the ground state energy and the effective mass of the polaron.

2 Theoretical model

We consider a quasi-two-dimensional quantum dot normal to the z axis. Therefore, we confine ourselves to considering only the motion of the electron in the x-y plane. The Hamiltonian of the electron-phonon system is given by

$$H = \frac{p^2}{2m} + V(\rho) + H_{ph} + H_{ph-e} + H_{SO}, \quad (1)$$

where the first term denotes the kinetic energy of the electron and the second term represents the confining potential in a single QD that is

$$V(\rho) = \frac{1}{2}m\omega_0^2\rho^2, \quad (2)$$

where m is the bare band mass of the electron and ω_0 is the confinement strength of the quantum dot.

The Hamiltonian of the phonons H_{ph} is given by

$$H_{ph} = \sum_{\mathbf{q}} \hbar\omega_{LO} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}}, \quad (3)$$

where $b_{\mathbf{q}}^{\dagger}$ ($b_{\mathbf{q}}$) is the creation (annihilation) operator of a bulk LO phonon with wave vector $q_1, \mathbf{q} = (\mathbf{q}_{//}, q_z)$.

The electron-phonon interaction term H_{ph-e} is expressed as

$$H_{ph-e} = \sum_{\mathbf{q}} [V_{\mathbf{q}} \exp(i\mathbf{q} \cdot \mathbf{r}) b_{\mathbf{q}} + h.c.], \quad (4)$$

where $\mathbf{r} = (\rho, z)$. The Fourier coefficient for the interaction are described by

$$V_q = i \left(\frac{\hbar \omega_{LO}}{q} \right) \left(\frac{\hbar}{2m\omega_{LO}} \right)^{1/4} \left(\frac{4\pi\alpha}{v} \right)^{1/2}, \quad (5a)$$

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{LO}} \right) \left(\frac{2m\omega_{LO}}{\hbar} \right)^{1/2} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right), \quad (5b)$$

where ϵ_∞ and ϵ_0 are the optical dielectric and the static dielectric constant. α is the electron-LO phonon coupling strength. v is the volume of the crystal.

The contribution of the Rashba effect to the single-electron Hamiltonian can be expressed as

$$H_{SO} = \frac{\alpha}{\hbar} (p_x \sigma_y - p_y \sigma_x) \quad (6)$$

where σ_x, σ_y , are the Pauli spin matrices and the Rashba parameter α_R is linearly dependent on the expectation value of the electric field $\langle E \rangle$. In semiconductor structures, it is determined by many factors such as the geometry [15]. $\alpha_R = c(E)$, there the coefficient c is inversely proportional to the energy gap and effective mass [16,17]. The Rashba interaction usually dominates in quantum dots obtain in a heterostructure [6,7,18]. We have chosen to include the Rashba term than the Dresselhaus term.

Following Tokuda [19], one also introduce the improved linear combination of the creation operator a_j^+ and annihilation operator a_j to represent the momentum and position of the electron in the x-y plane

$$p_j = \left(\frac{m\hbar\lambda}{2} \right)^{1/2} (a_j + a_j^+ + p_{0j}), \quad (7a)$$

$$\rho_j = i \left(\frac{\hbar}{2m\lambda} \right)^{1/2} (a_j - a_j^+), \quad (7b)$$

$$j = x, y \quad (7c)$$

where λ and p_0 are variational parameters. Carrying out a unitary transformation

$$U = \exp \left(\sum_{\mathbf{q}} (b_{\mathbf{q}}^+ f_{\mathbf{q}} - b_{\mathbf{q}} f_{\mathbf{q}}^*) \right) \quad (8)$$

where $f_{\mathbf{q}} (f_{\mathbf{q}}^*)$ is the variational parameter. The transformed Hamiltonian can be rewritten as

$$H' = H'_{||} + \frac{p_z^2}{2m} \quad (9)$$

The ground state wavefunction of the system is chosen as

$$|\Psi\rangle = |\varphi(Z)\rangle (a\chi_{\frac{1}{2}} + b\chi_{-\frac{1}{2}}) |0\rangle_b |0\rangle_a \quad (10)$$

where $|\varphi(Z)\rangle$ is the normalized electron wavefunction along the z direction and $|\langle \varphi(Z) | \varphi(Z) \rangle|^2 = \delta(Z)$ since the electrons are considered to be confined in an infinitesimally narrow layer. $\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ label the up and down states of the z component of

the spin, a and b are coefficients. $|0\rangle_a$ is the ground state of polaron, and $|0\rangle_b$ is the zero phonon state, which satisfied $b_q|0\rangle_b = a_j|0\rangle_a = 0$. To obtain the effective mass of strong-coupling polaron, the minimization of the energy should be performed by constraining the total momentum operator $\mathbf{P}_{||T}$ of the system parallel to the x-y plane. The total momentum of the system is parallel to the x-y plane operator can be represented as

$$\mathbf{P}_{||T} = \mathbf{P}_{||} + \sum_{\mathbf{q}} b_{\mathbf{q}}^+ b_{\mathbf{q}} \hbar \mathbf{q}_{||} \quad (11)$$

The minimization problem is now carried out by using the Lagrange multipliers, choosing an arbitrary constant multiplier. Now the ground state splitting energy of the whole system can be obtain as

$$E_{\pm} = \min [F_{\pm}(\mathbf{u}, \mathbf{p}_0, \lambda, f_{\mathbf{q}})] \quad (12)$$

$$F_{\pm}(\mathbf{u}, \mathbf{p}_0, \lambda, f_{\mathbf{q}}) = {}_a \langle 0 | {}_b \langle 0 | U^{-1} (H_{||} - \mathbf{p} \cdot \mathbf{u}) U | 0 \rangle_b | 0 \rangle_a \quad (13)$$

$F_{\pm}(u, \mathbf{p}_0, \lambda, f_{\mathbf{q}})$ may be called the variational parameter function. Using the variational method, we get the variational parameter $f_{\mathbf{q}}(f_{\mathbf{q}}^*)$ and \mathbf{p}_0 . Substituting $f_{\mathbf{q}}(f_{\mathbf{q}}^*)$ and \mathbf{p}_0 into F , we have

$$F_{\pm}(u, \lambda) = \frac{\hbar \lambda}{2} + \frac{\hbar \omega_0^2}{2\lambda} - \frac{mu^2}{2} - \frac{\alpha_R^2}{2\hbar^2} m \pm \frac{\alpha_R}{\hbar} mu - \frac{\alpha \hbar \sqrt{\lambda} \omega_{LO}^{1/2}}{\sqrt{\pi}} \left(1 + \frac{1}{3} \frac{u^2 m \lambda}{\hbar \omega_{LO}^2}\right) \quad (14)$$

Performing the variation of $F_{\pm}(u, \lambda)$ with respect to λ , we obtain the expression of the vibration frequency of strong-coupling polaron in a parabolic quantum dot

$$\lambda^2 - \alpha \sqrt{\frac{\omega_{LO}}{\pi}} \lambda^{\frac{3}{2}} - \omega_0^2 = 0 \quad (15)$$

By solving equation (15) we obtain the vibration frequency of the strong-coupling polaron

$$\lambda = \lambda_0 \quad (16)$$

Substituting these parameters and the function in equation (14), the ground state splitting energy of the strong-coupling polaron can be expressed as

$$E_{\pm} = \frac{\hbar \lambda_0}{2} + \frac{\hbar \omega_0^2}{2\lambda_0} - \frac{mu^2}{2} - \frac{\alpha_R^2}{2\hbar^2} m \pm \frac{\alpha_R}{\hbar} mu - \frac{\alpha \hbar \sqrt{\lambda_0} \omega_{LO}^{1/2}}{\sqrt{\pi}} \left(1 + \frac{1}{3} \frac{u^2 m \lambda_0}{\hbar \omega_{LO}^2}\right) \quad (17)$$

The spin-splitting energy at zero magnetic fields can be expressed as

$$E_{SO} = \pm \frac{\alpha_R}{\hbar} mu - \frac{\alpha_R^2}{2\hbar^2} m \quad (18)$$

For the momentum expectation value of the strong-coupling polaron in a parabolic quantum dot in the x-y plane, we find

$$\bar{\mathbf{P}}_{||=b} \langle 0|_a \langle 0|U^{-1} \mathbf{P}_{||T} U|0\rangle_a |0\rangle_b = m \left[1 \pm \frac{2\alpha_R}{\hbar u} + \frac{2\alpha}{3\sqrt{\pi}} \left(\frac{\lambda_0}{\omega_{LO}} \right)^{\frac{3}{2}} \right] u \quad (19)$$

It is evident from the structure of this expression that \mathbf{u} has the meaning of velocity which may be regarded as the average velocity of the polaron in the x-y plane, and the factor before \mathbf{u} , namely

$$m_{\pm}^* = m \left[1 \pm \frac{2\alpha_R}{\hbar \mathbf{u}} + \frac{2\alpha}{3\sqrt{\pi}} \left(\frac{\lambda_0}{\omega_{LO}} \right)^{\frac{3}{2}} \right] u \quad (20)$$

can be interpreted as the effective mass of the strong-coupling polaron in a parabolic quantum dot.

Finally, the effective Hamiltonian of strong-coupling polaron in a parabolic quantum dot can be expressed as

$$H_{eff} = H_{kin} + H_{int} \quad (21)$$

where

$$H_{kin} = \frac{\mathbf{p}_z^2}{2m} + \frac{\mathbf{p}_{||}^2}{2m^*} \quad (22)$$

$$H_{int} = \frac{\hbar\lambda_0}{2} + \frac{\hbar\omega_0^2}{2\lambda_0} - \frac{1}{\sqrt{\pi}} \alpha \hbar\omega_{LO} \left(\frac{\lambda_0}{\omega_{LO}} \right)^{\frac{1}{2}} - \frac{\alpha_R^2}{2\hbar^2} m \quad (23)$$

are the kinetic energy and the interaction energy of strong-coupling in a parabolic quantum dot.

From Eq. (20) one can see that the effective mass m_{\pm}^* of strong-coupling in a parabolic quantum dot depends not only on the frequency of phonon ω_{LO} and vibration frequency λ_0 but also on α_R the strength of spin-orbit coupling. From Eq. (23) one can see that the interaction energy H_{int} of strong-coupling in a parabolic quantum dot depends not only on the frequency of phonon ω_{LO} , the strength of confinement ω_0 , the vibration frequency λ_0 but also on α_R the strength of spin-orbit coupling.

3 Numerical results and discussion

To show more obviously the influence of α_R the strength of spin-orbit coupling, the vibration frequency λ_0 and the influence of the confinement strength ω_0 on the properties of strong coupling in a parabolic quantum dot, taking in a quantum dot of the RbCl crystal (the data for a RbCl crystal [20]: $\varepsilon_0 = 4.58$, $\varepsilon_{\infty} = 2.20$, $\hbar\omega_{LO} = 22.317$ meV, $\alpha = 3.81$, $\omega_{LO} = 3.39 \times 10^{13} \text{S}^{-1}$) for example, we perform a numerical evaluation.

Fig. 1 shows the relationships between polaron ground state energy $E_b = (\alpha_R = 0)$, ground state splitting energy E_{\pm} of the strong coupling in a parabolic quantum dot of the

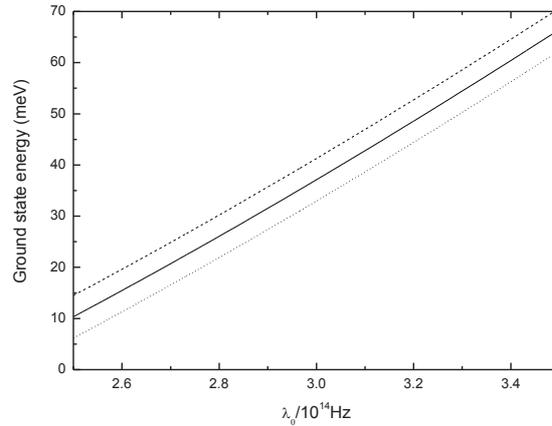


Figure 1: The polaron ground state energy $E_b = (\alpha_R = 0)$ and ground state splitting energy E_{\pm} calculated by using Eq. (17). Energy as a function of vibration frequency λ in the RbCl crystal. They are expressed by the black line, dash line respectively ($\alpha = 20$ meV nm, $u = 2 \times 10^4$ m/s).

RbCl crystal with the vibration frequency λ_0 . We assume that $\alpha_R = 20$ meV nm $u = 2 \times 10^4$ m/s. From the figure, one can see that polaron ground state energy E_b and ground state splitting energy E_{\pm} will increase strongly with increasing the vibration frequency λ_0 . The Rashba SO interaction originating from the lack of inversion symmetry which causes a local electric field perpendicular to the plane of heterostructure splits the ground state energy of the polaron into two branches, each of them is not stand for the splitting energy of polaron spin-up (spin-down) energy, but the result of common affect of polaron spin-up and spin-down. When the material selected, the increase α_R can be attributed to the increase in $\langle E \rangle$ by the negative gate voltage because it can not significantly charge the energy gap and effective mass, therefore, the coefficient can be treated as a constant. In another words, by applying a voltage to a gate the effective electric field in the conducting channel and thus the Rashba coupling parameter can be controlled. The Rashba parameter takes values in the range of $10^{-11} - 10^{-12}$ eV m [21]. When the splitting parameter α_R is very small, the spin splitting takes less than 1% of the polaron ground state energy. When the splitting parameter α_R is very large such as 20 meV nm the spin splitting energy is about $E_{SO} = 6.05$ meV. It takes about 6% of the polaron ground state energy. With the present of the phonons, the total energy of the partial is decreased, so the state of the polaron is much stable than electron's. Therefore, the splitting state of the polaron is much stable. Furthermore E_- state is the most stable in the splitting state of the polaron. So we can see that Rashba effect can not be neglected.

Fig. 2 shows the relationship between the confinement strength ω_0 and the vibration frequency λ_0 in RbCl crystal. We assume that $\alpha_R = 20$ meV nm. From the figure, one can see that polaron the confinement strength ω_0 will increase strongly with increasing the vibration frequency λ_0 . This is because of the exist of confining potential ω_0 limits the moving of electrons increase with increasing of the confining potential that is the

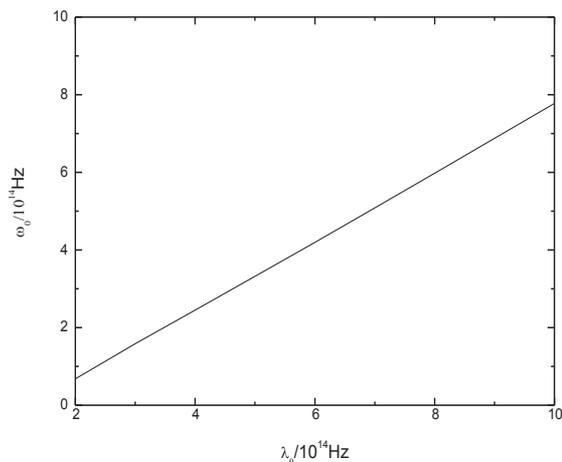


Figure 2: The confinement strength ω_0 as a function of the vibration frequency λ_0 in RbCl crystal which calculated by using Eq. (15).

decrease of ρ , the enhancement of the energy electron thermal motion which the medium is phonon and the interaction of electron-phonon enhance with diminishing the extent of particle's moving, cause the increase of the vibration frequency, so it shows the novel quantum size effect.

Fig. 3 shows the relationship between the vibration frequency λ_0 and the effective mass m_{\pm}^*/m in RbCl crystal. We assume that $\alpha_R=20 \text{ meV nm}$. From the figure, one can see that polaron the effective mass m_{\pm}^*/m will increase strongly with increasing the vibration frequency λ_0 . As we all know polaron is the interaction between electron and phoron,

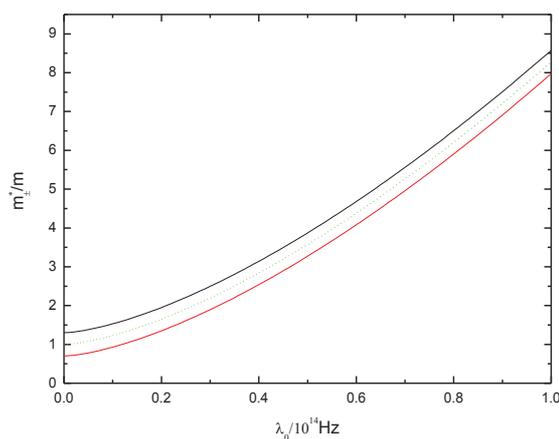


Figure 3: The effective mass m_{\pm}^*/m calculated by using Eq. (20). Effective mass as a function of the vibration frequency λ_0 in RbCl crystal.

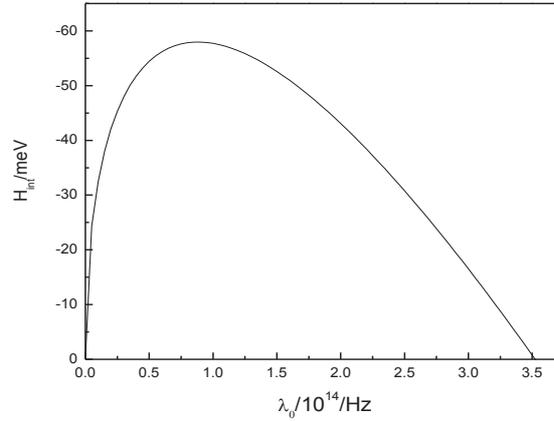


Figure 4: The interaction energy H_{int} calculated by using Eq. (23). Interaction energy as a function of the vibration frequency λ_0 in RbCl crystal.

which cause the effective mass of the electron changed. The Rashba SO interaction makes the density in the material of in different spin state, that is to say, spin state splits on their energies. This energy's split is the result of the split of the polaron's effective mass.

Fig. 4 shows the relationship between the interaction energy H_{int} and the vibration frequency λ_0 in RbCl crystal. From the figure, we can see that the interaction energy increases rapidly to the maximum $H_{intmax} = -58.06$ meV at $\lambda_0 = 0.8 \times 10^{14}$ Hz and decrease rapidly with increasing the λ_0 . We obtain $H_{int} = \hbar\lambda_0 - \frac{3}{2}a\hbar\sqrt{\frac{w_{LO}}{\pi}}\lambda_0^{1/2} - \frac{\alpha_k^2}{2\hbar^2}m$, after inserting Eq. (15) to Eq. (23). In the point of mathematical view, the increasing speed of λ is bigger than $\lambda^{\frac{1}{2}}$, but the coefficient of \hbar is smaller than $\frac{3}{2}a\hbar\sqrt{\frac{w_{LO}}{\pi}}$, so it appear the maximum. Inserting $\lambda_0 = 0.8 \times 10^{14}$ Hz (at the maximum point) into Eq. (15), ω_0 is obtained. $r_0 = (\frac{\hbar}{2m\omega_{LO}})^{\frac{1}{2}}$ is the radius of polaron and $l_0 = (\frac{\hbar}{m\omega_0})^{\frac{1}{2}}$ is the effective confinement length of the QD. We can find that $r_0 = l_0 = 1.3$ nm. It is said that, when the polaron's radius is equal to the effective confinement length of the QD, the interaction energy is the maximum. From that, we can draw the conclusion that interaction energy has sympathetic vibration character with the change of the confinement strength ω_0 , so felicitous confinement strength ω_0 is favor of stabilization of the polaron in semiconductor quantum dots.

4 Conclusion

In this paper, we have adopted improved liner combination operator method to investigate the ground state of a polaron which in the electron-LO phonon strong coupling region in a parabolic quantum dot by considering the influences of the Rashba SO interaction. The numerical calculation is performed on RbCl crystal. We find that the spin-

splitting energy and effective mass of polaron induced by Rashba SO interaction is sensitive to α_R the strength of spin-orbit coupling. The total polaronic correction is negative and decreases the ground state energy. The vibration frequency and the effective mass will increase with the confinement strength increasing. Whereas the interaction energy is sharply increased until the confinement strength reaches a certain value, then it will sharply decrease, so felicitous confinement strength ω_0 is favor of stabilization of the polaron in semiconductor quantum dots. From this paper, we can see that the Rashba effect plays a fundamental role in the understanding of the properties of the spin-dependent ground state energy of the polaron in semiconductor quantum dots.

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