Strong-coupling surface polaron in a magnetic field

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Abstract

By applying variational method, the strong electron-surface optical (SO) phonon interaction and the weak electron-longitudinal optical (LO) phonon interaction are studied systematically in present paper. The formula of induced energy $V_{e-so}$, $V_{e-lo}$ in both the ground and excited states are given. The numerical results show that as the distance between the electron and the polar crystal surface increases, the electron-LO phonon interaction energy increases yet the electron-SO phonon interaction energy decreases. The numerical results also show that both electron-LO and electron-SO phonon interaction are enhanced as the magnetic field strength increases.

Key words: Semiconductors, Electron-phonon interactions
1. Introduction

The behavior of polaron has received much attention in the past decades [1,2]. Huybrechts [3] proposed a linear combination operator method and investigated the property of polaron in strong electron-phonon coupling case. Tokuda [4] added another variational parameter to the momentum operator and studied the ground-state energy and effective mass of the bulk polaron. Gu [5] discussed the the ground-state energy, the first-excited state energy and the effective mass of intermediate-coupling polaron in a polaron slab. When external magnetic field is applied to the electron-phonon interaction system, the property of magnetopolaron attracted many investigators’ interests. Whitfield et al [6] studied the effectiveness of adiabatic approximation theory for a polaron in a magnetic field and they found that the usual adiabatic theory applied to a polaron in a strong magnetic field does not give the right weak coupling limit. Ercelebi [7] studied the two-dimensional magnetopolaron in the strong-coupling regime and proposed a modified coherent phonon state. Hai, Peeters et al [8] did research into the polaron-cyclotron-resonance spectrum resulting from interface- and slab-phonon modes in a GaAs/AlAs quantum well and an experiment was done to investigate the resonant magnetopolaron effects due to interface phonons in GaAs/AlGaAs multiple quantum well structures by Wang, Nickle et al [9]. Recently, the author etc have studied the electron self-energy and effective mass by the powerful Green’s function method [10].

For the bulk polaron, the perturbation theory is applicable when \( \alpha_l < 1 \) and the LLP (Lee-Low-Pines) variational method is effective when \( \alpha_l < 6 \). For the surface polaron, Pan [11] showed that when the electron-surface optical (SO) phonon coupling constant \( \alpha_s > 2.5 \), the strong coupling theory must be applied. Therefor, in some polar crystals, the weak electron-LO phonon coupling and strong electron-SO phonon coupling should be considered together. So far, the research work in such a field has been scarce.

In the present paper, using variational method and taking weak electron-LO phonon and strong electron-SO phonon interaction into account, we give the ground and excited states energies of the system, the electron-LO phonon interaction induced energy \( V_{e-LO} \) and the electron-SO phonon interaction induced energy \( V_{e-SO} \). Using polar crystal AgBr as an example, numerical evaluation are also presented.

2. Theory

Considering the following system: the semi-infinite space \( z > 0 \) is occupied by the AgBr
crystal, whereas the space \( z < 0 \) is a vacuum. The external magnetic field is applied along the \( z \) direction and an electron is moving in the polar crystal. \( \mathbf{B} = (0, 0, B) \), choosing the symmetric gauge for the vector potential, i.e. \( \mathbf{A} = B/2(-y, x, 0) \), the Hamiltonian describing an electron coupled to both LO phonons and SO phonons can be written as \( \hbar = m_b = 1 \), \( m_b \) is the band mass of the electron

\[
H = H_0 + H_\perp + H_{e-ph} = H_\perp + H_{/ /},
\]

\[
H_0 = \frac{P_\perp^2}{2} + \frac{\omega^2}{8}(x^2 + y^2) + \frac{\omega_e}{2}L_z + \sum_k \omega_{lo}a_k^\dagger a_k + \sum_q \omega_{so}b_q^\dagger b_q,
\]

\[
H_\perp = \frac{P_z^2}{2} + \frac{e^2}{4z\varepsilon_\infty(\varepsilon_\infty + 1)},
\]

\[H_{e-ph} = H_{e-lo} + H_{e-so},\]

\[H_{e-lo} = \sum_k [V^*_k \sin(zk_z)\exp(-ik_{//} \cdot \rho)a_k^\dagger + h.c.],\]

\[H_{e-so} = \sum_q [V^*_q \exp(-qz)\exp(-iq \cdot \rho)b_q^\dagger + h.c.].\]

where

\[
V^*_k = i\left(\frac{4\pi e^2\omega_{lo}}{\varepsilon V}\right)^{\frac{1}{2}}k, \quad \frac{1}{\varepsilon} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}.
\]

\[
V^*_q = i\left(\frac{\pi e^2\omega_{so}}{\varepsilon^* qA}\right)^{\frac{1}{2}}, \quad \frac{1}{\varepsilon^*} = \frac{\varepsilon_0 - 1}{\varepsilon_0 + 1} - \frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 1}.
\]

In the above equations, \( a_k^\dagger (a_k) \) is the creation(annihilation) operator of bulk LO phonons with three-dimensional wave vector \( k \), \( b_k^\dagger (b_k) \) is the corresponding operator for the SO phonons with two-dimensional wave vector \( q \). \( P_{//} = (p_x, p_y) \) and \( \rho = (x, y) \) are the electron momentum and position vector in xy plane, respectively, and \( p_z \) is the electron momentum in z direction. \( k_{//} = (k_x, k_y) \) is phonon wave vector in the xy plane. \( \omega_{lo} \) and \( \omega_{so} \) are the frequencies of the bulk LO and SO phonons. \( \varepsilon_0 \) and \( \varepsilon_\infty \) are the static and high-frequencies dielectric constant of the crystal respectively. \( A \) and \( V \) are the surface area and the volume of the crystal.

The polaron system wave function can be separated into the electron and the phonon parts.

\[
|\psi\rangle = |\phi_e\rangle|\phi_{ph}\rangle
\]

With \( |\phi_{ph}\rangle = u_1 u_2 |0\rangle \), \(|0\rangle \) is the phonon ground state, and the explicit form of \( u_1, u_2 \) will be introduced in the following.
Let us start from the unitary transformation:

\[ u_1 = \exp(-i (\sum_k a_1 a_1^\dagger a_k k_{//} \cdot \rho + \sum_q a_2 b_q^\dagger b_q \cdot \rho )) \]  

(8)

With \( a_1 = 1 \) and \( a_2 = 0 \) corresponding to the weak-coupling limit case and the strong-coupling limit case respectively. The parts of polaron Hamiltonian can be transformed into:

\[ H'_0 = u_1^{-1} H_0 u_1 = \frac{1}{2} (P_{//} - \sum_k a_k a_k^\dagger) + \frac{\omega_c^2}{8} (x^2 + y^2) + \frac{\omega_c}{2} L_z \]

\[ + \frac{\omega_c}{2} \sum_k a_k^\dagger (yk_x - xk_y) + \sum_k \omega_{lo} a_k^\dagger a_k + \sum_q \omega_{so} b_q^\dagger b_q , \]  

(9)

\[ H'_{e-so} = u_1^{-1} H_{e-so} u_1 = \sum_q [V^*_q \exp(-qz) \exp(-iq \cdot \rho) \rho \cdot \rho + h.c.] , \]  

(10)

\[ H'_{e-so} = u_1^{-1} H_{e-so} u_1 = H \]  

(12)

Following the scheme of Huybrechts, we introduce the creation and annihilation operators \( c_j^\dagger \) and \( c_j \) by

\[ p_j = \frac{\sqrt{\lambda}}{2} (c_j^\dagger + c_j) , \]

(13)

\[ \rho_j = \frac{i}{\sqrt{\lambda}} (c_j - c_j^\dagger) . \]

(14)

Where the subscript \( j \) refers to the \( x \) and \( y \) directions, \( \lambda \) is the variational parameter, and \( c_j^\dagger (c_j) \) is Boson operator.

Rewriting (9), (11) using (13), (14), one gets:

\[ H'_0 = \frac{\lambda}{8} \left( \sum_j (c_j^\dagger c_j^\dagger c_j + c_j c_j c_j^\dagger) + \sum_j (c_j^\dagger c_j + c_j c_j^\dagger) \right) - \frac{\sqrt{\lambda}}{2} \sum_{k,j} a_k^\dagger a_k k_{//} (c_j^\dagger + c_j) \]

\[ + \frac{1}{2} \sum_k a_k^\dagger a_k k_{//}^2 + \frac{1}{2} \sum_{k,k'} a_k^\dagger a_{k'}^\dagger a_k a_{k'} k_{//} k_{//}' + \frac{\omega_c^2}{8\lambda} \sum_j (c_j^\dagger c_j + c_j c_j^\dagger) \]

\[ - \frac{\omega_c^2}{8\lambda} \sum_j (c_j^\dagger c_j^\dagger + c_j c_j) + \frac{i\omega_c}{2} (c_y c_y^\dagger - c_x c_x^\dagger) + \sum_k \omega_{lo} a_k^\dagger a_k + \sum_q \omega_{so} b_q^\dagger b_q \]

\[ + \frac{i\omega_c}{2\sqrt{\lambda}} \sum_k a_k^\dagger a_k [k_x (c_y^\dagger - c_y) - k_y (c_x^\dagger - c_x)] , \]  

(15)

\[ H'_{e-so} = \sum_q [V^*_q \exp(-qz) \exp(\sum_j \frac{q_j}{\sqrt{\lambda}} (c_j - c_j^\dagger)) b_q^\dagger + h.c.] , \]  

(16)
Yet, $H'_{e-lo}$ and $H'_{\perp}$ are invariable in forms. Let continue to do the $u_2$ transformation:

$$u_2 = \exp[\sum_k (a_k^+ f_k e^{-ikx/\rho_0} - a_k f_k^* e^{ikx/\rho_0}) + \sum_q (b_q^+ g_q e^{-iq\rho_0} - b_q g_q^* e^{iq\rho_0})]$$  \hspace{1cm} (17)

Where $f_k(f_k^*)$ and $g_q(g_q^*)$ are variational parameters, and $\rho_0 = (x_0, y_0)$ is the electron orbit center where $x_0 = x/2 - p_y/\omega_c$, $y_0 = y/2 + p_x/\omega_c$. The necessity of making the phonon deformation centered at $\rho_0$ was emphasized in an elaborate discussion by Whitfield et al [6].

$$u_2^{-1} a_k u_2 = a_k + f_k e^{-ikx/\rho_0}, \quad u_2^{-1} a_k^\dagger u_2 = a_k^\dagger + f_k^* e^{ikx/\rho_0}, \quad (18)$$

$$u_2^{-1} b_q u_2 = b_q + g_q e^{-iq\rho_0}, \quad u_2^{-1} b_q^\dagger u_2 = b_q^\dagger + g_q^* e^{iq\rho_0} \quad . \quad (19)$$

Performing $u_2$ transformation and using (18) and (19), one can get $H_o''$, $H'_{e-lo}$ and $H'_{e-so}$ after lengthy calculation.

(1) The ground state:

Determining the ground state $|0\rangle$ in the new representation by

$$c_j |0\rangle = a_k |0\rangle = b_q |0\rangle = 0$$  \hspace{1cm} (20)

one gets the energy $E''_{ji}(0)$ of the ground state

$$E''_{ji}(0) = <H''_{ji}> = <H''_0 + H''_{e-lo} + H''_{e-so}>$$

$$= \frac{\lambda}{4} + \frac{\omega^2}{4\lambda} + \sum_k \omega_{lo} |f_k|^2 + \sum_q \omega_{so} |g_q|^2 + \frac{1}{2} \sum_k |f_k|^2 k_{ji}^2 + \frac{1}{2} \sum_{k,k'} |f_k|^2 |f_{k'}|^2 k \cdot k'$$

$$+ \sum_k [V_k^* \sin(zk_z) f_k^* + V_k \sin(zk_z) f_k] \exp(-\frac{k_{ji}^2}{8}(\frac{1}{\lambda} + \frac{\lambda}{\omega^2_c}))$$

$$+ \sum_q [V_q^* \exp(-qz) g_q^* + V_q \exp(-qz) g_q] \exp(-\frac{q^2}{8}(\frac{1}{\lambda} + \frac{\lambda}{\omega^2_c})). \quad (21)$$

Minimizing $E''_{ji}(0)$ with respect to $f_k(f_k^*)$ and $g_q(g_q^*)$ and neglecting higher order of $f_k$, one gets

$$E''_{ji}(0) = \frac{\lambda}{4} + \frac{\omega^2}{4\lambda} + V_{e-lo}(0) + V_{e-so}(0)$$  \hspace{1cm} (22)

Where $V_{e-lo}(0)$ and $V_{e-so}(0)$ are the correction energy induced by electron-LO phonon and electron-SO phonon interaction respectively, with

$$V_{e-lo} = - \sum_k |V_k|^2 \sin^2(zk_z) \exp(-\frac{k_{ji}^2}{4}(\frac{1}{\lambda} + \frac{\lambda}{\omega^2_c}), \quad (23)$$
\[ V_{e-s0} = -\sum_q \frac{|V_q|^2 \exp(-2qz) \exp\left(-\frac{q^2}{4}\left(\frac{1}{\lambda} + \frac{1}{\omega^2}\right)\right)}{\omega_{so}}. \] (24)

Considering the explicit forms of \( V_k \) and \( V_q \), (23) and (24) can be reduced to

\[ V_{e-lo} = -\frac{\sqrt{2\alpha l\omega_{lo}}}{2} \int_0^\infty \left(1 - e^{-2k_z^2}\right) \exp\left(-\frac{k^2_z}{4}\left(\frac{1}{\lambda} + \lambda\omega^2\right)\right) \frac{dk_z}{1 + \frac{k^2_z}{2\omega_{lo}}}, \] (25)

\[ V_{e-so} = -\frac{\sqrt{2\alpha_s\omega_{so}}}{2} \int_0^\infty \exp(-2qz) \exp\left(-\frac{q^2}{4}\left(\frac{1}{\lambda} + \frac{1}{\omega^2}\right)\right) dq. \] (26)

In eq.(22), if neglecting \( V_{e-lo}(0), V_{e-so}(0) \) and minimizing \( E''_{//}(0) \) with respect to \( \lambda \), one can obtain \( \lambda = \omega_c \) and \( E''_{//}(0) = \frac{1}{2}\omega_c \). Obviously, this is the electron ground state energy of Landau Level.

The effective Hamiltonian of the polaron system in the ground state \( H_{eff} \) is

\[ H_{eff} = E''_{//}(0) + H_\perp = \frac{p_z^2}{2} + \frac{\lambda}{4} + \frac{\omega^2}{4\lambda} + V_{e-lo} + V_{e-so} + V_{img}, \] (27)

with

\[ V_{img} = \frac{\epsilon^2(\varepsilon_\infty - 1)}{4\varepsilon_\infty + 1}. \]

(2) The excited state:

The excited state \( |1> \) in the new representation is

\[ |1> = c_j^\dagger |0> = a_k^\dagger |0> = b_q^\dagger |0> \] (28)

considering

\[ <1|\exp(-iq \cdot \rho_0)|1> = \exp\left(-\frac{q^2}{8\lambda} - \frac{\lambda q^2}{8\omega^2_c}\right) \left[1 - \left(\frac{q^2}{8\lambda} + \frac{\lambda q^2}{8\omega^2_c}\right)^2\right] \] (29)

similarly, one gets

\[ E''_{//}(1) = \frac{3\lambda}{4} + \frac{3\omega^2}{4\lambda} + \omega_{lo} + \omega_{so} + V_{e-lo}(1) + V_{e-so}(1) \] (30)

Where \( V_{e-lo}(1) \) and \( V_{e-so}(1) \) are the correction energy induced by electron-LO phonon and electron-SO phonon interaction of the excited state respectively, with

\[ V_{e-lo}(1) = -\sum_k |V_k|^2 \sin^2(\nu z) \exp\left(-\frac{k^2_z}{4}\left(\frac{1}{\lambda} + \lambda\omega^2\right)\right) \left[1 - \left(\frac{k^2_z}{8\lambda} + \frac{\lambda k^2_z}{8\omega^2_c}\right)^2\right], \] (31)

\[ V_{e-so}(1) = -\sum_q |V_q|^2 \exp(-2qz) \exp\left(-\frac{q^2}{4}\left(\frac{1}{\lambda} + \lambda\omega^2\right)\right) \left[1 - \left(\frac{q^2}{8\lambda} + \frac{\lambda q^2}{8\omega^2_c}\right)^2\right] \omega_{so}. \] (32)
3. Discussion and Conclusion

Taking the polaron in polar crystal AgBr as an example, we perform a numerical evaluation. The parameters concerned are listed as follows: \( \varepsilon_0 = 10.6, \varepsilon_\infty = 4.68, \hbar \omega_{lo} = 17.1 \text{meV}, \hbar \omega_{so} = 14.5 \text{meV}, \alpha_l = 1.56, \alpha_s = 2.56, m_b = 0.22m, \) \( m \) is the free electron mass. All the above parameters are taken from [12].

Fig.1 Fig.2

Fig.1 shows the relationships between the induced potential \(|V_{e-lo}(0)|\) resulting from the electron-LO phonon interaction, the induced potential \(|V_{e-so}(0)|\) resulting from electron-SO phonon interaction, and their sum \(|V_{e-lo}(0)|+|V_{e-so}(0)|\) and the coordinate \( z \). From fig.1 we can see that the induced potential \( V_{e-lo}(0) \) increase with increasing coordinate \( z \), whereas \( V_{e-so}(0) \) decrease with increasing coordinate \( z \). Compared with the weak electron-phonon interaction case [13], \( |V_{e-so}(0)| \) and \( |V_{e-lo}(0)| \) are larger than the corresponding weak coupling ones, yet their lines tendency is similar to the weak coupling ones. When \( z < 10 \text{Å} \), \( |V_{e-so}(0)| \) is larger than \( |V_{e-lo}(0)| \), whereas for \( z > 35 \text{Å} \), \( |V_{e-so}(0)| \) becomes smaller compared with \( |V_{e-lo}(0)| \) and so \( |V_{e-lo}(0)| \) is the dominant term. \( |V_{e-lo}(0)|+|V_{e-so}(0)| \) decreases with increasing \( z \). When \( z > 35 \text{Å} \), \( |V_{e-lo}(0)|+|V_{e-so}(0)| \) approaches \( |V_{e-lo}(0)| \) because \( |V_{e-so}(0)| \) is much smaller compared with \( |V_{e-lo}(0)| \).

Fig.2 shows the induced potentials as a function of the electron coordinate \( z \) for different magnetic fields. In fig.2, the dot-line stands for the case when \( B=4 \text{T} \) and the solid-line stands for the \( B=8 \text{T} \) case. From fig.2, we can see that \( |V_{e-lo}(0)| \) and \( |V_{e-so}(0)| \) for \( B=8 \text{T} \) are larger than the corresponding ones for \( B=4 \text{T} \). This result show that external magnetic field can enhance the interaction between an electron and phonons. Let us give a possible physical explanation of the result. When magnetic field is applied, the polarizability of the crystal increases and the density of phonons increases. Because the strength of the electron-phonon interaction is proportional to the number of phonons, the interaction energies, for both \( |V_{e-lo}(0)| \) and \( |V_{e-so}(0)| \), increase with increasing magnetic field strength.
Fig. 3 illustrates the energy difference induced by the electron-LO (SO) phonon interaction between the excited and ground states. From Fig. 3 one can see that the difference between $V_{e-so}(1)$ and $V_{e-so}(0)$ decreases, yet the difference between $V_{e-lo}(1)$ and $V_{e-lo}(0)$ increases as the coordinate $z$ increases. As $z$ is small ($z < 10\text{Å}$) the magnitude of $V_{e-so}(1) - V_{e-so}(0)$ is much large than that of $V_{e-lo}(1) - V_{e-lo}(0)$, and when $z > 33\text{Å}$ $|V_{e-so}(1) - V_{e-so}(0)|$ becomes less than $|V_{e-lo}(1) - V_{e-lo}(0)|$. These results give further implication that the electron-SO phonon interaction play a dominant role as electron are near the polar crystal surface.

In summary, by applying variational method, the strong electron-surface optical (SO) phonon interaction and the weak electron-longitudinal optical (LO) phonon interaction are studied systematically in present paper. The formula of induced energies $V_{e-so}(0), V_{e-lo}(0), V_{e-so}(1), V_{e-lo}(1)$ are given. The numerical results show that as the distance between the electron and the polar crystal surface increases, the electron-LO phonon interaction energy increases yet the electron-SO phonon interaction energy decreases. The numerical results also show that both electron-LO and electron-SO phonon interaction are enhanced as the magnetic field strength increases.
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Figure Captions

Fig.1. $|V_{e-so}(0)|$, $|V_{e-lo}(0)|$, and $|V_{e-so}(0)| + |V_{e-lo}(0)|$ as a function of coordinate $z$.

Fig.2. $|V_{e-so}(0)|$ and $|V_{e-lo}(0)|$ as a function of coordinate $z$ for different magnetic fields. The solid line and the dot line represent $B=8T$ and $B=4T$, respectively.

Fig.3 $|V_{e-ph}(1) - V_{e-ph}(0)|$ as a function of coordinate $z$ at $B=10T$. 
$B = 10 \text{ T}$

$|V_{\text{eso}}(1) - V_{\text{eso}}(0)|$

$|V_{\text{eso}}(1) - V_{\text{eso}}(0)|$

$Z \times 10^{-10} \text{ m}$