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POLARON IN POLAR CRYSTAL INTERFACE IN ELECTRIC FIELD①

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ABSTRACT With the help of linear composed operators of electronic momentum and coordination the effect of electric field on interface polaron is studied in this paper. The reciprocal radius, ground state energy and effective mass of interface polaron were calculated. When the direction of electric field is from the crystal with larger dielectric constant to the crystal with smaller dielectric constant, appling electric field is favorable to form interface polaron. Analytics and numerical results are given, respectively, in this paper for weak and moderate electric field. These results are helpful for explaining the behavior of interface polaron in the electric field.

Key words polaron interface polar crystal ground state energy

1 INTRODUCTION

Electron in solid state material has important effect on its thermal, electric and magnetic properties. The interaction between electron and lattice has received increasing attention. In recent years polaron theory has succeeded in explaining not only the electric conductivity of electric conduction macromolecular materials, but also the electron behavior and transport mechanism of semiconductor[1]. In polar crystal electron property strongly depends on the interaction electron and LO phonon. However, on the surface (or interface) it is necessary to take into account the influence of SO-phonons[2-4].

Binding energy, screen constant and effective mass, on which electric conductivity depends, are important parameters describing electron state in crystal. It is often carried out in electro-magnetic field to determine the parameters mentioned above, however electromagnetic field has strong effect on them, hence it is very meaningful to clarify the change of the parameters in electromagnetic field. Recently Liang Xixia[5] reported the behavior of interface polaron in magnetic field. The author of this paper[6] studied the properties of weak coupling interface polaron in electric field. In this paper, we will further study the effect of electric field on strong coupling interface polaron.

Method applied was linear composed operators of electron momentum and coordinator proposed by Huybrechts[6], which is adapted to surface (or interface) polaron[2]. The remainder of this paper was organized as following: In sec. 2, we will give the Hamiltonian and variation function of interface polaron in electric field. This is followed by the calculation results of ground state energy, effective and reciprocal radius of interface polaron and some discussion in sec. 3, and concluding remark is given in sec. 4.

2 HAMILTONIAN AND VARIATION FUNCTION OF SYSTEM

We consider a system constituted by a junction of two semi-infinite polar ionic crystals with a interface at $z = 0$ and characterized by the lattice state, optical dielectric constant ε_{01}, $\varepsilon_{\infty 1}$ for $z > 0$ and ε_{02}, $\varepsilon_{\infty 2}$ for $z < 0$, respectively, a static external electric field is applied perpendicular to the interface. The Hamiltonian can be

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written as

$$H = \frac{p_{\parallel}^2}{2m_{\parallel}^*} + \frac{p_z^2}{2m_z^*} + \frac{e^2}{4z}\frac{\varepsilon_{\infty 1} - \varepsilon_{\infty 2}}{\varepsilon_{\infty 1}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})} - ez\mathscr{E}_{ex} + \sum h\omega_q a_q^+ a_q + \sum_a h\omega_s a_Q^+ a_Q + \sum_q V_q \sin q_z z \exp(i\boldsymbol{q}_{\parallel} \cdot \rho)(a_q + a_{-q}^+) + \sum_Q V_Q \exp(-Qz + i\boldsymbol{Q} \cdot \rho)(a_Q + a_{-Q}^+) \quad (1)$$

The first and second term in Eq. (1) are the kinetic energy of quasi-free electron, the third image potential energy; the fifth and sixth are the contribution of bulk LO phonon and SO phonon; and the fourth, seventh, eighth interaction are electron-electric field, bulk LO phonon, SO phonon, respectively, where

$$|V_q|^2 = \frac{4\pi\alpha(h\omega_0)^2}{L^3 q^2 \beta_0},$$

$$\alpha_{\text{I}} = \frac{e^2}{h}\left|\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}}\right|\left(\frac{m_{\parallel}^*}{2h\omega_0}\right)^{1/2}$$

$$\beta_0 = \left(\frac{2m^*\omega_0}{h}\right)^{1/2}$$

$$|V_Q|^2 = \frac{2\pi\alpha_s(h\omega_s)^2}{L^2 Q\beta_s} \cdot \frac{2\varepsilon_{01}\varepsilon_{\infty 1}}{(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})(\varepsilon_{01} + \varepsilon_{02})},$$

$$\alpha_s = \frac{e^2}{h}\left(\frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}}\right)\left(\frac{m_{\parallel}^*}{2h\omega_s}\right)^{1/2},$$

$$\beta_s = \left(\frac{2m_{\parallel}^*\omega_s}{h}\right)^{1/2}$$

where α is Frölich electron-phonon coupling constant. For ionic crystal the interaction of electron-phonon is very strong, i. e α is large, the detail of all terms see Ref[7].

For the main effect of external electric field on electron state is in z direction, we introduce the linear combined operators of electronic momentum and coordinator[6] on x-y plane:

$$\begin{cases} p_j = \left(\frac{m_{\parallel}^* h\lambda}{2}\right)^{1/2}(b_j + b_j^+ + p_{0j}) \\ \rho_j = i\left(\frac{h}{2m_{\parallel}^*\lambda}\right)^{1/2}(b_j - b_j^+) \end{cases}$$

$$j = 1, 2 \quad (2)$$

where b_j, b_j^+ are Boson operators; p_{0j} is variational parameter determined by minimizing the ground state energy.

However in this variation the conservation condition of interface polaron momentum must be considered. In strong coupling we apply variation technique developed by Lee, Low, and Pine and the following wave function

$$\boldsymbol{P}_{\parallel} = \boldsymbol{p}_{\parallel} + \sum_q h\boldsymbol{q}_{\parallel} a_q^+ a_q + \sum_Q h\boldsymbol{Q}_{\parallel} a_Q^+ a_Q \quad (3)$$

$$|\Phi\rangle = U|\Psi(z), 0\rangle \quad (4)$$

where $U = \exp[\sum_q (a_q^+ f_q - a_q f_q^*) + \sum_Q (a_Q^+ f_Q - a_Q f_Q^*)]$, $|0\rangle$ is the vaccume state of phonon and polaron, i. e $a_q|0\rangle = a_Q|0\rangle = b_j|0\rangle = 0$, λ, p_{0j}, f_q and f_Q are variational parameters.

Thus the variation function of the system is as follows:

$$\mathscr{H} = \langle \Psi(z)|\left(\frac{h\lambda}{2} + \frac{h\lambda}{4}p_0^2 + \frac{p_z^2}{2m_z^*} + \frac{e^2}{4z}\frac{\varepsilon_{\infty 1} - \varepsilon_{\infty 2}}{\varepsilon_{\infty 1}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})} - ez\mathscr{E}_{ex} - \left(\frac{m_{\parallel}^* h\lambda}{2}\right)^{1/2}\boldsymbol{p}_0 \cdot \boldsymbol{u}_{\parallel} + \sum_Q V_Q \exp\left(-Qz - \frac{hQ^2}{4m_{\parallel}^*\lambda}\right)(f_Q + f_Q^*) + \sum_q V_q \sin q_z z \exp\left(-\frac{hq_{\parallel}^2}{4m_{\parallel}^*\lambda}\right)(f_q + f_q^*) + \sum h\omega_s|f_Q|^2 + \sum_Q h\omega_0|f_q|^2 - \sum h\boldsymbol{Q}_{\parallel} \cdot \boldsymbol{u}_{\parallel}|f_Q|^2 - \sum h\boldsymbol{q}_{\parallel} \cdot \boldsymbol{u}_{\parallel}|f_q|^2\right)|\Psi(z)\rangle \quad (5)$$

3 GROUND STATE ENERGY

We determine the variational parameters f_q, f_Q and p_0 by minimizing Eq. (5). The vector $\boldsymbol{u}_{\parallel}$ is Lagrange multiplier and the polaron velocity. For low temperature by using slow velocity approximation, we neglect the effect of $\boldsymbol{u}_{\parallel}$ in variation of determining λ, by variating Eq. (5) for the λ we can get following equation meeted by parameter λ

$$\bar{\lambda}^{1/2} = \left(\frac{\lambda}{\omega_0}\right)^{1/2} = \frac{\sqrt{\pi}}{4}\alpha\left(1 + \frac{4}{\sqrt{\pi}}(A_1 - 0.5)g\right) \quad (6)$$

where

$$A_1 = \frac{2\varepsilon_{01}\varepsilon_{\infty 1}}{(\varepsilon_{01}+\varepsilon_{02})(\varepsilon_{\infty 1}+\varepsilon_{\infty 2})}$$

$$g = \langle \Psi(z) | \int_0^{\infty} \exp(x^2 - 2xz(\frac{2m_{\parallel}^{*}\lambda}{h})^{1/2})\mathrm{d}x | \Psi(z) \rangle$$

Substituting wave function (4) into Hamiltonian (1), and then getting the ground state energy of the system:

$$E = \langle \Phi | H | \Phi \rangle = \frac{\mathscr{P}_{\parallel}^2}{2M_{\parallel}^{*}} + \langle \Psi(z) | \{\frac{p_z^2}{2m_z^{*}} + \frac{e^2}{4z}\frac{\varepsilon_{\infty 1}-\varepsilon_{\infty 2}}{\varepsilon_{\infty 1}(\varepsilon_{\infty 1}+\varepsilon_{\infty 2})} - ez\mathscr{E}_{ex}\} | \Psi(z) \rangle - \frac{\pi}{32}\alpha^2 h\omega_0 (1+\frac{4}{\pi}(A_1 - 0.5)g)^2 \quad (7)$$

where $\mathscr{P}_{\parallel}$ is the expectation value of the momentum of interface polaron, and $M_{\parallel}^{*}$ is its effective mass, They are given by $\mathscr{P}_{\parallel} = \langle \Phi | \boldsymbol{P}_{\parallel} | \Phi \rangle = M_{\parallel}^{*}\boldsymbol{u}_{\parallel}$, Assuming $|\Psi(z)\rangle$ in the form

$$|\Psi(z)\rangle = \begin{cases} 2\zeta^{3/2} z e^{-\zeta z} & z \geqslant 0 \\ 0 & z < 0 \end{cases} \quad (8)$$

where ζ is another constant determined by ground state energy miniming, and then g can be approximately written as

$$g = 4\zeta^3 \int_0^{\infty}\int_0^{\infty} z^2 e^{-2\zeta z} e^{-x^2 - 2xz(\frac{2m_{\parallel}^{*}\lambda}{h})^{1/2}} \mathrm{d}y\mathrm{d}z \approx 4\zeta^3 \cdot \int_0^{\infty} \frac{z e^{-2\zeta z}\mathrm{d}z}{2(\frac{2m_{\parallel}^{*}\lambda}{h})^{1/2}} = 0.5\zeta' \overline{\lambda}^{1/2}$$

Under the approximation, Finishing the calculation in Eq. (7) can get ground state energy of interface polaron. An equation met by reciprocal radius ζ can be obtained by minimizing the ground state energy:

$$(1-\frac{4}{\pi}(A_1 - 0.5))\zeta'^3 - \frac{\alpha}{4}(A_1 - A_2 - 0.5)\zeta'^2 + \frac{3}{4}\frac{e\mathscr{E}_{ex}}{\beta_0 h\omega_0} = 0 \quad (9)$$

where $A_2 = \frac{\varepsilon_{01}(\varepsilon_{\infty 1}-\varepsilon_{\infty 2})}{(\varepsilon_{01}-\varepsilon_{\infty 1})(\varepsilon_{\infty 1}+\varepsilon_{\infty 2})}$, $\zeta' = \zeta/\beta_0$. The final term in eq. (9) is the effect of external electric field. Without electric field the reciprocal radius of interface polaron becomes:

$$\zeta' = \zeta'_0 = \frac{\alpha(A_1 - A_2 - 0.5)}{4(1-\frac{4}{\pi}(A_1 - 0.5))} \quad (10)$$

The condition of $\zeta' > 0$ asks for $\varepsilon_{\infty 1} < \varepsilon_{\infty 2}$, this means that interface polaron can only exist in the dielectric with smaller optical dielectric constant. The ground state energy of interface polaron becomes:

$$E' = E'_0 = \frac{\mathscr{P}_{\parallel}^2}{2M_{\parallel}^{*}} - \frac{\pi}{32}\alpha^2 - \frac{\alpha^2}{16}\frac{(A_1 - A_2 - 0.5)^2}{(1-\frac{4}{\pi}(A_1 - 0.5))^2} \quad (11)$$

where $E' = E/h\omega_0$. When external field is weak, ζ', E' and $M_{\parallel}^{*}$ are as following, respectively

$$\zeta' = \zeta'_0 - \frac{3}{4}\frac{e\mathscr{E}_{ex}}{\zeta_0'^2\beta_0 h\omega_0} - \frac{9}{8}\frac{e^2\mathscr{E}_{ex}^2}{\zeta_0'^5\beta_0^2 h^2\omega_0^2} \quad (12)$$

$$E' = E'_0 - \frac{3}{2}\frac{e\mathscr{E}_{ex}}{\zeta'_0\beta_0 h\omega_0} - \frac{9}{16}(1-\frac{2}{\pi}(A_1 - 0.5)^2)\frac{e^2\mathscr{E}_{ex}^2}{\zeta_0'^4\beta_0^2 h^2\omega_0^2} \quad (13)$$

$$M_{\parallel}^{*} = m_{\parallel}^{*}(1+\frac{\pi^4}{128}\alpha + \frac{3}{64}\alpha^4(A_1 - 0.5)\zeta_0'^2 - \frac{9}{64}\alpha^3(A_1 - 0.5)\frac{e\mathscr{E}_{ex}}{\zeta_0'^2\beta_0 h\omega_0} - \frac{19}{128}\alpha^3(A_1 - 0.5)\cdot\frac{e^2\mathscr{E}_{ex}^2}{\zeta_0'^5\beta_0^2 h^2\omega_0^2} \quad (14)$$

We can see from Eqs. (12) ~ (14), when electric field is very weak, ζ' and E'_0 decrease with electric field. So appling an electric field whose direction is from the dielectric with larger ε_{∞} to the dielectric with smaller ε_{∞} is favourable to form interface polaron, and the fact that effective mass decreases with electric field shows that electron-electric field interaction weakens electron-phonon coupling. If the direction is reverse, it is harmful to interface polaron. For the moderate electric field, the numerical

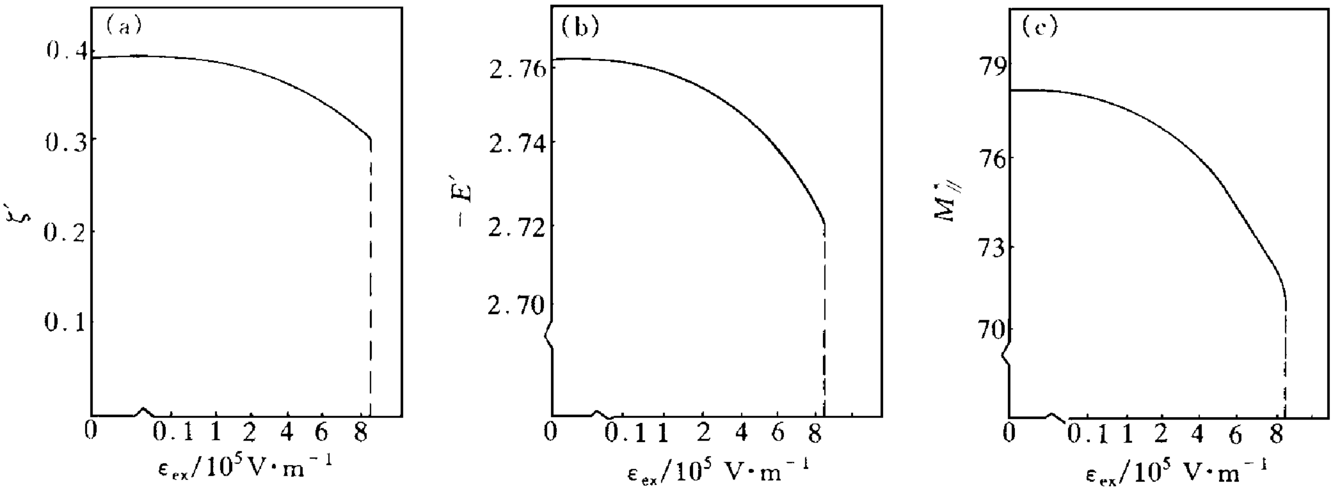

Fig. 1 The dependance interface polaron state for interface RbBr-LiF in electric field

(a) —reciprocal radius; (b) —ground state energy; (c) —effective mass

calculating results are presented in Fig. 1 for interface whichare composed of crystals RbBr and LiF.

Fig. 1 shows the effect of electric field on interface polaron. When electric field is smaller than 10^4 V/m, the effect is so small that it can be negleted. When electric field gradually grows, the electron-electric field interaction becomes obvious, it is shown that the reciprocal raduies ζ, ground state energy E_0 and effective mass $M^*_{\parallel}$ decrease fast when electric field increases. When electric field reaches some critical value (for RbBr-LiF interface, the value is 8.125 × 10^5 V/m), $\zeta' = 0$, the electron-phonon coupling is replaced by electron-electric field interaction, the electron in dielectric look like free electron, these show that the dielectric is punctured in the electric field.

4 CONCLUSIONS

(1) Interface polaron can only exist in the dielectric with small optical dielectric constant, it is identical with the conclusion given by Ref. [2].

(2) The effect of electric field on interface polaron can be divided into three stages: when electric field is smaller than 10^4 V/m, the effect is so small that it can be neglected; when electric field is between 10^4 V/m and the critical electric fields, the effect gradully grows, electron-phonon coupling weakens, and binding energy decreases; when electric field is larger than critical electric field, electron-electric field interaction makes electron become free electron.

(3) When the direction of electric field is from the dielectric with larger ε_∞ to the dielectric with smaller ε_∞, appling electric field is favourable to form interface polaron. If the direction of electric field is converted, it is unfavourable to form interface polaron.

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