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强耦合表面极化子的激发能量

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摘要: 采用线性组合算符方法及幺正变换方法研究了电子与表面光学(SO)声子和体纵光学(LO)声子均为强耦合的表面极化子的激发态性质。计算了体系的有效哈密顿量、振动频率和体系由基态向第一激发态跃迁所需的激发能量。

关 键 词: 强耦合; 表面极化子; 激发能量
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1 引 言

20 世纪 70 年代初, Ibach[1] 在 ZnO 等半导体的表面成功地完成了低能电子衍射实验, 该实验的成功引起了人们对表面极化子理论研究的浓厚兴趣。Sak[2] 和 Evans[3] 对表面极化子进行了系统的研究。国内外许多学者[4~7] 也在这方面作了不少工作, 取得了可喜成绩。80 年代, 顾世洧及其合作者[8] 对半无限晶体中弱、中耦合极化子进行了讨论。顾等[9] 又对强耦合极化子作了进一步的讨论。但是以往的研究仅限于对体系基态性质的研究, 而对体系处于激发态性质的研究较少。

Huybrechts[10] 用线性组合算符法引入两个变分参量研究了体纵光学极化子的内部激发态性质。Gifeisman[11] 用微扰法讨论了半导体的第一激发态波函数。Lepine[12] 采用 Matz 和 Burkey 的福克近似方法计算了束缚 Fröhlich 极化子的激发态能量。Devreese[13] 通过引进一个新的变分函数, 讨论了束缚极化子的激发态能量。Lu 等[14] 采用有效质量近似变分方法计算了在极性晶体膜中极化子的基态和第一激发态能量。Qin 等[15] 用格林函数方法研究了极性晶体膜中极化子的自陷能、基态和激发态能量的温度依赖性。Sahoo[16] 利用变分运算得到多维极性晶体基态和激发态的能量。Chun 等[17] 利用 Landau 和 Pekar 变分法计算了氢杂质在柱面量子线的基态和激发态的束缚能量。但是采用 Huybrechts 方法研究极化子的内部激发态性质的甚少[18]。本文采用幺正变换方法和线性组合算符法研究了在强耦合情况下表面极化子的有效哈密顿量、振动频率及体系由基态向第一激发态跃迁所需要的激发能量。

2 理 论

设所考虑的晶体位于 x-y 平面内, 表面法线方向在 z 轴上, 在 $z>0$ 的半无限空间里充满着极性晶体, 晶体内的电子在表面附近运动(距表面 $z>0$), 则电子–声子系哈密顿量可写为

$$H=\frac{P_{\parallel}^{2}}{2m}+\frac{P_{z}^{2}}{2m}+\frac{e^{2}(\varepsilon_{\infty}-1)}{4z\varepsilon_{\infty}(\varepsilon_{\infty}+1)}+\sum_{\vec{Q}}\hbar\omega_{S}b_{\vec{Q}}^{+}b_{\vec{Q}}+\sum_{\vec{W}}\hbar\omega_{L}a_{\vec{W}}^{+}a_{\vec{W}}+\sum_{\vec{Q}}\left[e^{-Qz}\left(V_{Q}^{*}e^{-i\vec{Q}\cdot\vec{\rho}}b_{\vec{Q}}^{+}+h\cdot c\right)\right]+\sum_{\vec{W}}\left[\sin(W_{z}z)\left(V_{W}^{*}e^{-i\vec{W}_{\parallel}\cdot\vec{\rho}}a_{\vec{W}}^{+}+h\cdot c\right)\right] \tag{1a}$$

其中

$$V_{W}^{*}=i\left(\frac{4\pi e^{2}\hbar\omega_{L}}{\bar{\varepsilon}V}\right)^{1/2} \tag{1b}$$

$$V_{Q}^{*}=i\left(\frac{\pi e^{2}\hbar\omega_{S}}{\varepsilon^{*}S}\right)^{1/2} \tag{1c}$$

$$\frac{1}{\bar{\varepsilon}}=\frac{1}{\varepsilon_{\infty}}-\frac{1}{\varepsilon_{0}},\quad \frac{1}{\varepsilon^{*}}=\frac{\varepsilon_{0}-1}{\varepsilon_{0}+1}-\frac{\varepsilon_{\infty}-1}{\varepsilon_{\infty}+1} \tag{1d}$$

$$\omega_{S}^{2}=\frac{1}{2}(\omega_{T}^{2}+\omega_{L}^{2}) \tag{1e}$$

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$$\alpha_S=\frac{me^2}{\varepsilon^*\hbar^2 u_S}\qquad \alpha_L=\frac{me^2}{\varepsilon\hbar^2 u_L} \tag{1f}$$

$$u_S=\left(\frac{2m\omega_S}{\hbar}\right)^{1/2}\quad u_L=\left(\frac{2m\omega_L}{\hbar}\right)^{1/2}\quad u_\lambda=\left(\frac{2m\lambda}{\hbar}\right)^{1/2} \tag{1g}$$

式中各量物理意义与文献[19]相同。

把体系的哈密顿量分成平行和垂直于晶体表面的两部分

$$H=H_{\parallel}+H_{\perp} \tag{2a}$$

$$H_{\perp}=\frac{P_z^2}{2m}+\frac{e^2(\varepsilon_\infty-1)}{4z\varepsilon_\infty(\varepsilon_\infty+1)} \tag{2b}$$

$$H_{\parallel}=\frac{P_{\parallel}^2}{2m}+\sum_{\vec W}\hbar\omega_L a_{\vec W}^+a_{\vec W}+\sum_{\vec Q}\hbar\omega_S b_{\vec Q}^+b_{\vec Q}+\sum_{\vec W}\left[\sin(W_z z)(V_W^* e^{-i\vec W_{\parallel}\cdot\vec\rho}a_{\vec W}^+ + h\cdot c)\right]+\sum_{\vec Q}\left[e^{-Qz}(V_Q^* e^{-i\vec Q\cdot\vec\rho}b_{\vec Q}^+ + h\cdot c)\right] \tag{2c}$$

由于电子在 z 方向的运动是缓慢的, 所以当确定电子在 x-y 平面内运动状态时, 可以把 z 方向的坐标和动量看成参量, 这种方法通常称为准绝热近似, 所以处理 x-y 平面运动时, 将 z, P_z 看成参量。

对电子横向运动的动量和坐标引进线性组合算符

$$P_j=\left(\frac{m\hbar\lambda}{2}\right)^{1/2}(B_j+B_j^+) \tag{3a}$$

$$j=x,\ y$$

$$\rho_j=i\left(\frac{\hbar}{2m\lambda}\right)^{1/2}(B_j-B_j^+) \tag{3b}$$

这里 λ 为变分参量。

作两次幺正变换

$$U_1=\exp\left[-\left(ia_1\sum_{\vec W}a_{\vec W}^+a_{\vec W}\vec W_{\parallel}+ia_2\sum_{\vec Q}b_{\vec Q}^+b_{\vec Q}\vec Q\right)\cdot\vec\rho\right] \tag{4a}$$

$$U_2=\exp\left[\sum_{\vec W}(a_{\vec W}^+f_W-a_{\vec W}f_W^*)+\sum_{\vec Q}(b_{\vec Q}^+g_Q-b_{\vec Q}g_Q^*)\right] \tag{4b}$$

其中 $f_W(f_W^*)$, $g_Q(g_Q^*)$ 为变分参量。

考虑表面极化子动量守恒的对称性, 则有

$$\left\langle\frac{P_{\parallel}^2}{2m}\right\rangle=\left\langle\sum_W\sum_j\frac{\hbar W_{\parallel j}P_{\parallel j}}{2m}|f_W|^2\right\rangle=\left\langle\sum_Q\sum_j\frac{\hbar Q_jP_{\parallel j}}{2m}|g_Q|^2\right\rangle=\left\langle\frac{1}{2m}\left(\sum_W\hbar\vec W_{\parallel}|f_W|^2\right)^2\right\rangle=\left\langle\frac{1}{2m}\left(\sum_Q\hbar\vec Q|g_Q|^2\right)^2\right\rangle=\frac{1}{2}\hbar\lambda \tag{5}$$

变换后体系的哈密顿量为

$$H_{\parallel}''=U_2^{-1}U_1^{-1}H_{\parallel}U_1U_2=$$

$$\frac{\hbar\lambda}{2}\sum_j B_j^+B_j+\frac{\hbar\lambda}{2}(1-a_1)^2+\frac{\hbar\lambda}{2}(1-a_2)^2-\frac{\hbar\lambda}{2}+\sum_{\vec W}\left(\hbar\omega_L+a_1^2\frac{\hbar^2W_{\parallel}^2}{2m}\right)(a_{\vec W}^++f_{\vec W}^*)(a_{\vec W}+f_{\vec W})+\sum_{\vec Q}\left(\hbar\omega_S+a_2^2\frac{\hbar^2Q^2}{2m}\right)(b_{\vec Q}^++g_{\vec Q}^*)(b_{\vec Q}+g_{\vec Q})+\sum_{\vec W}\sin(W_z z)\left[V_W^*(a_{\vec W}^++f_W^*)\exp\left(-\frac{\hbar}{4m\lambda}(1-a_1)^2W_{\parallel}^2\right)\right]\cdot$$

$$\exp\left[-(1-a_1)\left(\frac{\hbar}{2m\lambda}\right)^{1/2}\sum_j W_{\parallel j}B_j^+\right]\cdot\exp\left[(1-a_1)\left(\frac{\hbar}{2m\lambda}\right)^{1/2}\sum_j W_{\parallel j}B_j\right]+h\cdot c\Big]+$$

$$\sum_{\vec Q}e^{-Qz}\left(V_Q^*(b_{\vec Q}^++g_Q^*)\exp\left(-\frac{\hbar}{4m\lambda}(1-a_2)^2Q^2\right)\right)\cdot\exp\left[-(1-a_2)\left(\frac{\hbar}{2m\lambda}\right)^{1/2}\sum_j Q_jB_j^+\right]\cdot\exp\left[(1-a_2)\left(\frac{\hbar}{2m\lambda}\right)^{1/2}\sum_j Q_jB_j+h\cdot c\right]+H_1'' \tag{6}$$

(6) 式中 H_1'' 为剩余项, 因不重要可忽略。

取 $|0\rangle_a|0\rangle_b|0\rangle_B$ 为基态尝试波函数, $|0\rangle_a|0\rangle_b|1\rangle_B$ 为第一激发态尝试波函数, 利用

$$a_{\vec W}|0\rangle_a=a_{\vec Q}|0\rangle_b=B_j|0\rangle_B=0$$

$$B_j^+|0\rangle_B=|1\rangle_B \tag{7}$$

则有

$$\mathscr{H}_{\parallel}^0={}_B\langle 0|{}_b\langle 0|{}_a\langle 0|H_{\parallel}'|0\rangle_a|0\rangle_b|0\rangle_B=$$

$$\frac{\hbar\lambda}{2}(1-a_1)^2+\frac{\hbar\lambda}{2}(1-a_2)^2-\frac{\hbar\lambda}{2}+\sum_W\left(\hbar\omega_L+a_1^2\frac{\hbar^2W_{\parallel}^2}{2m}\right)|f_W|^2+\sum_Q\left(\hbar\omega_S+a_2^2\frac{\hbar^2Q^2}{2m}\right)|g_Q|^2+\sum_W\sin(W_z z)\left[V_W^*f_W^*\exp\left(-\frac{\hbar}{4m\lambda}(1-a_1)^2W_{\parallel}^2\right)+h\cdot c\right]+$$

$$\sum_Q e^{-Qz}\left[V_Q^* g_Q^* \exp\left(-\frac{\hbar}{4m\lambda}(1-a_2)^2Q^2\right)+h\cdot c\right] \quad (8)$$

利用变分技术得 $f_W(f_W^*)$、$g_Q(g_Q^*)$，代入上式得

$$\mathscr{H}^0_{\|} = \frac{\hbar\lambda}{2}(1-a_1)^2+\frac{\hbar\lambda}{2}(1-a_2)^2-\frac{1}{2}\hbar\lambda- \sum_W \frac{|V_W|^2\sin^2(Wz)\exp\left[-\frac{\hbar}{2m\lambda}(1-a_1)^2W_\|^2\right]}{\hbar\omega_L+a_1^2\frac{\hbar^2W_\|^2}{2m}} - \sum_Q \frac{|V_Q|^2e^{-2Qz}\exp\left[-\frac{\hbar}{2m\lambda}(1-a_2)^2Q^2\right]}{\hbar\omega_s+a_2^2\frac{\hbar^2Q^2}{2m}} \quad (9)$$

令

$$t_1=\frac{1-a_1}{a_1}\sqrt{\frac{\omega_L}{\lambda}} \quad (10a)$$

$$t_2=\frac{1-a_2}{a_2}\sqrt{\frac{\omega_s}{\lambda}} \quad (10b)$$

将(10)式代入(9)式有

$$\mathscr{H}^0_{\|} = \frac{\hbar\lambda}{2}\frac{1}{\left(1+\frac{1}{t_1}\sqrt{\frac{\omega_L}{\lambda}}\right)^2}+\frac{\hbar\lambda}{2}\frac{1}{\left(1+\frac{1}{t_2}\sqrt{\frac{\omega_s}{\lambda}}\right)^2}-\frac{\hbar\lambda}{2}-\alpha_L\hbar\omega_L t_1\left(1+t_1\sqrt{\frac{\lambda}{\omega_L}}\right)\left[\frac{\sqrt{\pi}}{2}\frac{e^{t_1^2}}{t_1}\mathrm{erfc}\,\frac{1}{2}(t_1)-f_1(z)\right]-\alpha_S\hbar\omega_S t_2\left(1+t_2\sqrt{\frac{\lambda}{\omega_S}}\right)f_2(z) \quad (11a)$$

这里

$$f_1(z)=\int_0^\infty\frac{\exp\left\{-x^2-2zu_L\left[\left(\frac{\lambda}{\omega_L}\right)^{\frac{1}{2}}+\frac{1}{t_1}\right]x\right\}}{x^2+t_1^2}\mathrm{d}x \quad (11b)$$

$$f_2(z)=\int_0^\infty\frac{\exp\left\{-y^2-2zu_s\left[\left(\frac{\lambda}{\omega_s}\right)^{\frac{1}{2}}+\frac{1}{t_2}\right]y\right\}}{y^2+t_2^2}\mathrm{d}y \quad (11c)$$

同理

$$\mathscr{H}^1_{\|} = {}_B\langle 1|\,{}_b\langle 0|\,{}_a\langle 0|H''_{\|}|0\rangle_a|0\rangle_b|1\rangle_B = \frac{\hbar\lambda}{2}(1-a_1)^2+\frac{\hbar\lambda}{2}(1-a_2)^2- \sum_W \frac{|V_W|^2\sin^2(Wz)\exp\left[-\frac{\hbar}{2m\lambda}(1-a_1)^2W_\|^2\right]}{\hbar\omega_L+a_1^2\frac{\hbar^2W_\|^2}{2m}}\cdot\left[1-(1-a_1)^2\frac{\hbar W_\|^2}{2m\lambda}\right]- \sum_Q \frac{|V_Q|^2e^{-2Qz}\exp\left[-\frac{\hbar}{2m\lambda}(1-a_2)^2Q^2\right]}{\hbar\omega_s+a_2^2\frac{\hbar^2Q^2}{2m}}\cdot\left[1-(1-a_2)^2\frac{\hbar Q^2}{2m\lambda}\right] \quad (12)$$

将(10)式代入(12)式得

$$\mathscr{H}^1_{\|} = \frac{\hbar\lambda}{2}\frac{1}{\left(1+\frac{1}{t_1}\sqrt{\frac{\omega_L}{\lambda}}\right)^2}+\frac{\hbar\lambda}{2}\frac{1}{\left(1+\frac{1}{t_2}\sqrt{\frac{\omega_s}{\lambda}}\right)^2}-\alpha_L\hbar\omega_L t_1\left(1+t_1\sqrt{\frac{\lambda}{\omega_L}}\right)\left\{(1+t_1^2)\left(\frac{\pi}{2}\frac{e^{t_1^2}}{t_1}\mathrm{erfc}(t_1)\right)-f_1(z)+\frac{\sqrt{\pi}}{2}\left(\exp z^2u_L^2\left(\left(\frac{\lambda}{\omega_L}\right)^{\frac{1}{2}}+\frac{1}{t_1}\right)^2\mathrm{erfc}\left(zu_L\left(\left(\frac{\lambda}{\omega_L}\right)^{\frac{1}{2}}+\frac{1}{t_1}\right)-1\right)\right)\right\}-\alpha_s\hbar\omega_s t_2\left(1+t_2\sqrt{\frac{\lambda}{\omega_s}}\right)\left\{(1+t_2^2)f_2(z)-\frac{\sqrt{\pi}}{2}\exp z^2u_s^2\left(\left(\frac{\lambda}{\omega_s}\right)^{\frac{1}{2}}+\frac{1}{t_2}\right)^2\cdot\mathrm{erfc}\left(zu_s\left(\left(\frac{\lambda}{\omega_s}\right)^{\frac{1}{2}}+\frac{1}{t_2}\right)\right)\right\} \quad (13)$$

对电子-SO 声子、电子-LO 声子均为强耦合时，满足条件 $a_1\to0$, $a_2\to0$ ($t_1\to\infty$, $t_2\to\infty$)，将此条件代入(13)式有

$$\mathscr{H}^0_{\|} = \frac{\hbar\lambda}{2}\left(1-\frac{2}{t_1}\sqrt{\frac{\omega_L}{\lambda}}+\frac{3}{t_1^2}\frac{\omega_L}{\lambda}\right)+\frac{\hbar\lambda}{2}\left(1-\frac{2}{t_2}\sqrt{\frac{\omega_s}{\lambda}}+\frac{3}{t_2^2}\frac{\omega_s}{\lambda}\right)-\frac{1}{2}\hbar\lambda-\frac{\sqrt{\pi}}{2}\alpha_L\hbar\omega_L\sqrt{\frac{\lambda}{\omega_L}}\left(1-e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)\right)-\frac{\sqrt{\pi}}{2}\alpha_L\hbar\omega_L\left(1-e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)\right)\frac{1}{t_1}-\alpha_L\hbar\omega_L\sqrt{\frac{\lambda}{\omega_L}}\left(-\frac{\sqrt{\pi}}{4}+\frac{\sqrt{\pi}}{4}\mathrm{erfc}(zu_\lambda)e^{z^2u_\lambda^2}-\frac{1}{2}zu_\lambda+\frac{\sqrt{\pi}}{2}z^2u_\lambda^2\mathrm{erfc}(zu_\lambda)e^{z^2u_\lambda^2}\right)\frac{1}{t_1^2}-\frac{\sqrt{\pi}}{2}\alpha_s\hbar\omega_s\sqrt{\frac{\lambda}{\omega_s}}e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)-\frac{\sqrt{\pi}}{2}\alpha_s\hbar\omega_s e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)\frac{1}{t_2}+\alpha_s\hbar\omega_s\sqrt{\frac{\lambda}{\omega_s}}\left(\frac{\sqrt{\pi}}{4}\mathrm{erfc}(zu_\lambda)e^{z^2u_\lambda^2}-\frac{1}{2}u_\lambda z+\frac{\sqrt{\pi}}{2}z^2u_\lambda^2\mathrm{erfc}(zu_\lambda)e^{z^2u_\lambda^2}\right)\frac{1}{t_2^2} \quad (14)$$

将(14)式变分得到

$$\lambda^{1/2}=\frac{1}{2}\alpha_L\pi^{1/2}\omega_L^{1/2}+(\alpha_s\sqrt{\omega_s}-\alpha_L\sqrt{\omega_L})\cdot\left[(1+2u_\lambda^2z^2)\frac{\sqrt{\pi}}{2}\mathrm{erfc}(zu_\lambda)e^{u_\lambda^2z^2}-u_\lambda z\right] \quad (15)$$

$$t_1=\frac{3\omega_L+2\alpha_L\sqrt{\omega_L\lambda}\left(\frac{\sqrt{\pi}}{4}+\frac{1}{2}u_\lambda z\right)}{\sqrt{\lambda\omega_L}+\frac{\sqrt{\pi}}{2}\alpha_L\omega_L\left(1-e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)\right)}-\frac{2\alpha_L\left(-\frac{\sqrt{\pi}}{4}\mathrm{erfc}(zu_\lambda)e^{z^2u_\lambda^2}+\frac{\sqrt{\pi}}{2}z^2u_\lambda^2\mathrm{erfc}(zu_\lambda)e^{u_\lambda^2}\right)}{\sqrt{\lambda\omega_L}+\frac{\sqrt{\pi}}{2}\alpha_L\omega_L\left(1-e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)\right)} \quad (16a)$$

$$t_2=\frac{3\omega_s-\alpha_s\sqrt{\omega_s\lambda}u_\lambda z}{\sqrt{\lambda\omega_s}+\frac{\sqrt{\pi}}{2}\alpha_s\omega_s e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)}+\frac{2\alpha_s\sqrt{\omega_s\lambda}\left(\frac{\sqrt{\pi}}{4}\mathrm{erfc}(zu_\lambda)e^{z^2u_\lambda^2}+\frac{\sqrt{\pi}}{2}z^2u_\lambda^2\mathrm{erfc}(zu_\lambda)e^{z^2u_\lambda^2}\right)}{\sqrt{\lambda\omega_s}+\frac{\sqrt{\pi}}{2}\alpha_s\omega_s e^{z^2u_\lambda^2}\mathrm{erfc}(zu_\lambda)} \quad (16b)$$

由(15)式可得

$$\lambda=\lambda_0(z) \quad (17)$$

同理将 $a_1(a_2)\to 0$, $t_1(t_2)\to\infty$ 及(17)式代入(14)式有

$$\begin{aligned}
\mathscr{H}_{\parallel}^{1}=&\frac{E\lambda_0}{2}\left(1-\frac{2}{t_1}\sqrt{\frac{\omega_L}{\lambda_0}}+\frac{3}{t_1^2}\frac{\omega_L}{\lambda_0}\right)+\frac{E\lambda_0}{2}\left(1-\frac{2}{t_2}\sqrt{\frac{\omega_s}{\lambda_0}}+\frac{3}{t_2^2}\frac{\omega_s}{\lambda_0}\right)-\\
&\alpha_L E\omega_L\left(\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_L}}-\frac{1}{2}\sqrt{\frac{\lambda_0}{\omega_L}}zu_{\lambda_0}-\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_L}}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})+\frac{\sqrt{\pi}}{2}\sqrt{\frac{\lambda_0}{\omega_L}}z^2u_{\lambda_0}^2\mathrm{erfc}(zu_{\lambda_0})e^{z^2u_{\lambda_0}^2}\right)-\\
&\alpha_L E\omega_L\left(\frac{\sqrt{\pi}}{4}-\frac{1}{2}u_{\lambda_0}z-\frac{\sqrt{\pi}}{4}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})+\frac{\sqrt{\pi}}{2}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)\frac{1}{t_1}-\\
&\alpha_L E\omega_L\left(-\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_L}}-\frac{1}{2}\sqrt{\frac{\lambda_0}{\omega_L}}u_{\lambda_0}z+\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_L}}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})+\frac{\sqrt{\pi}}{2}\sqrt{\frac{\lambda_0}{\omega_L}}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)\frac{1}{t_1^2}-\\
&\alpha_s E\omega_s\left(\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_s}}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})+\frac{1}{2}\sqrt{\frac{\lambda_0}{\omega_s}}zu_{\lambda_0}-\frac{\sqrt{\pi}}{2}\sqrt{\frac{\lambda_0}{\omega_s}}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)-\\
&\alpha_s E\omega_s\left(\frac{1}{2}u_{\lambda_0}z+\frac{\sqrt{\pi}}{4}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})-\frac{\sqrt{\pi}}{2}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)\frac{1}{t_2}-\\
&\alpha_s E\omega_s\left(\frac{1}{2}\sqrt{\frac{\lambda_0}{\omega_s}}u_{\lambda_0}z-\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_s}}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})-\frac{\sqrt{\pi}}{2}\sqrt{\frac{\lambda_0}{\omega_s}}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)\frac{1}{t_2^2}
\end{aligned} \quad (18)$$

根据准绝热近似理论得到体系处于基态的有效哈密顿量为

$$\mathscr{H}_{\mathrm{eff}}^{0}=\frac{P_z^2}{2m}+\frac{e^2(\varepsilon_\infty-1)}{4z\varepsilon_\infty(\varepsilon_\infty+1)}+\mathscr{H}_{\parallel}^{0} \quad (19)$$

体系处于第一激发态的有效哈密顿量为

$$\mathscr{H}_{\mathrm{eff}}^{1}=\frac{P_z^2}{2m}+\frac{e^2(\varepsilon_\infty-1)}{4z\varepsilon_\infty(\varepsilon_\infty+1)}+\mathscr{H}_{\parallel}^{1} \quad (20)$$

则体系由基态跃迁到第一激发态的激发能量

$$\begin{aligned}
\Delta E=&\mathscr{H}_{\mathrm{eff}}^{1}-\mathscr{H}_{\mathrm{eff}}^{0}\\
=&\frac{E\lambda}{2}-\alpha_L E\omega_L\left(-\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_L}}+\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_L}}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})-\frac{1}{2}\sqrt{\frac{\lambda_0}{\omega_L}}zu_{\lambda_0}+\frac{\sqrt{\pi}}{2}\sqrt{\frac{\lambda_0}{\omega_L}}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)-\\
&\alpha_L E\omega_L\left(-\frac{\sqrt{\pi}}{4}+\frac{\sqrt{\pi}}{4}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})-\frac{1}{2}zu_{\lambda_0}+\frac{\sqrt{\pi}}{2}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)\frac{1}{t_1}-\\
&\alpha_s E\omega_s\left(-\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda_0}{\omega_s}}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})+\frac{1}{2}\sqrt{\frac{\lambda_0}{\omega_s}}zu_{\lambda_0}-\frac{\sqrt{\pi}}{2}\sqrt{\frac{\lambda_0}{\omega_s}}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)-\\
&\alpha_s E\omega_s\left(-\frac{\sqrt{\pi}}{4}e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})+\frac{1}{2}zu_{\lambda_0}-\frac{\sqrt{\pi}}{2}z^2u_{\lambda_0}^2e^{z^2u_{\lambda_0}^2}\mathrm{erfc}(zu_{\lambda_0})\right)\frac{1}{t_2}
\end{aligned} \quad (21)$$

3 结果与讨论

为进一步理论分析，下面就两种极限情形分别讨论。

1. 当极化子离表面十分近，即 $z\ll u_L^{-1}$(或 u_S^{-1})时，有

$$t_1=\frac{3\omega_L}{\sqrt{\lambda\omega_L}} \quad (22a)$$

$$t_2=\frac{3\omega_S+\frac{\sqrt{\pi}}{2}\alpha_S\sqrt{\omega_S\lambda}}{\sqrt{\lambda\omega_S}+\frac{\sqrt{\pi}}{2}\alpha_S\omega_S} \quad (22b)$$

$$\sqrt{\lambda}=\frac{1}{2}\alpha_S\sqrt{\omega_S\pi} \quad (22c)$$

激发能量

$$\Delta E=\frac{\pi}{4}\alpha_S^2E\omega_S+\frac{\frac{\pi}{2}\alpha_S^2}{6+\frac{\pi}{2}\alpha_S^2}E\omega_S \quad (23)$$

(23) 式所得结果与电子仅与表面光学声子强耦合时所得激发能量完全一致。由(22c) 式和(23) 式可以看出振动频率 λ 和激发能量 ΔE 只与表面光学声子有关, 振动频率和激发能量随电子-SO 声子耦合常数 α_S 及 SO 声子频率 ω_S 的增加而增大。

2. 当极化子远离表面, 即 $z \gg u_L^{-1}$ (或 u_S^{-1}) 时, 有

$$t_1 = \frac{3\omega_L + 2\alpha_L\sqrt{\omega_L\lambda}\left(\frac{\sqrt{\pi}}{4} - \frac{1}{4zu\lambda}\right)}{\sqrt{\lambda\omega_L} + \frac{\sqrt{\pi}}{2}\alpha_L\omega_L\left(1 - \frac{1}{\sqrt{\pi}zu\lambda}\right)} \tag{24a}$$

$$t_2 = \frac{3\omega_S + \frac{1}{2}\alpha_S\frac{\sqrt{\omega_S\lambda}}{zu\lambda}}{\sqrt{\lambda\omega_S} + \frac{1}{2}\alpha_S\frac{\omega_S}{zu\lambda}} \tag{24b}$$

$$\sqrt{\lambda} = \frac{1}{2}\alpha_L\sqrt{\pi\omega_L} + \frac{1}{2}\left(\alpha_S\sqrt{\pi\omega_S} - \alpha_L\sqrt{\pi\omega_L}\right)\frac{1}{zu\lambda} \tag{24c}$$

激发能量

$$\Delta E = \frac{1}{2}E\lambda - \alpha_L E\omega_L\left(-\frac{\sqrt{\pi}}{4}\sqrt{\frac{\lambda}{\omega_L}} + \frac{1}{4}\sqrt{\frac{\lambda}{\omega_L}}\frac{1}{zu\lambda}\right) - \alpha_L E\omega_L\left(-\frac{\sqrt{\pi}}{4} + \frac{1}{4zu\lambda}\right)\frac{1}{t_1} + \alpha_S E\omega_S\sqrt{\frac{\lambda}{\omega_S}}\frac{1}{4zu\lambda} + \alpha_S E\omega_S\frac{1}{4zu\lambda}\frac{1}{t_2} \tag{25}$$

由(24) 和(25) 式可知, 当电子远离表面时, 体系的振动频率 λ, 激发能量 ΔE 不仅与 SO 声子和 LO 声子有关, 而且还与距离晶体表面的深度 Z 有关, 但 SO 声子的影响远小于 LO 声子的影响, 当 $z \to \infty$ 时, 有

$$t_1 = \frac{3\omega_L + \frac{\sqrt{\pi}}{2}\alpha_L\sqrt{\omega_S\lambda}}{\sqrt{\lambda\omega_L} + \frac{\sqrt{\pi}}{2}\alpha_S\omega_L} \tag{26a}$$

$$t_2 = \frac{3\omega_S}{\sqrt{\lambda\omega_S}} \tag{26b}$$

$$\sqrt{\lambda} = \frac{\pi}{2}\alpha_S\sqrt{\omega_L} \tag{26c}$$

$$\Delta E = \frac{\pi}{4}\alpha_L^2 E\omega_L + \frac{\frac{\pi}{2}\alpha_S^2}{6 + \frac{\pi}{2}\alpha_S^2}E\omega_S \tag{26d}$$

由上式可以看出, 振动频率 λ 和激发能量 ΔE 只与 LO 声子有关, 与 SO 声子无关。且振动频率和激发能量随 α_L 和 ω_L 的增加而增大。

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The Excitation Energy of the Strong Coupling Surface Polaron

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Abstract: In the early 1970's Ibach has made low energy electron diffracting (LEED) experiments on ZnO and other semiconductor surfaces. The surface polaron in crystals have been of considerable interest. Sak and Evans studied theoretically the surface polaron in polar crystals. In the 1980's Gu *et al*. discussed the weak and intermediate coupling surface polaran in semi-infinite crystals. Gu *et al*. investigated further the strong coupling surface polaron. In fact, so far research of the surface polaron only was restricted to the calculation of ground state energy.

Huybrechts studied the properties of the internal excited state of the optical polaron by using the linear combination operator method. Gifeisman *et al*. calculated the wave functions of first excited state using perturbation theory. The excited state energy of bound Fröhlich polaron was evaluated using the Fock approximation of Matz and Burkey by Lepine. A new variational wave function to describe the ground state and the excited states of a bound polaron is proposed by Devreese. Using the effective-mass approximation and the variational method the ground-state and first-excited state energy of a polaron in a polar-crystal slab, due to the interactions of the electron with the BO and SO phonons, are calculated self-consistently by Lu and Li. Qin and Gu investigate temperature dependence of the electron self-energy in the polar-crystal slab using Green-function method. In calculation, they consider the effect of the excited states on the electron self-energy and find the ground-state energy be about 11% lower than that of bulk polaron. A variational calculation is performed by Sahoo to obtain the ground state and the first excited state of the Fröhlich bipolaron in a multidimensional polar crystal. Chun *et al*. discussed the hydrogenic impurity binding energy of the ground and the excited state in a cylindrical quantum wire by using Landau and Pekar variational method. However, using a Huybrechts's method, the properties of internal excited state of the polaron has not been investigated so far.

In this paper, the effective Hamiltonian, the vibration frequency and the excitation energy of strong coupling surface polaron are calculated by using the linear combination operator and unitary transformation methods. Two limiting cases of coordinate z are discussed. The results show that for strong-coupling surface polaron the excitation energy will increase with increasing the electron-phonon coupling constant $\alpha_S(\alpha_L)$ and the vibrational frequency of phonon $\omega_S(\omega_L)$.

Key words: strong-coupling; surface polaron; excitation energy

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