固体讨论班

Spin Orbital Coupling

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CONTENTS

I. PREFACE

The purpose of this lecture is trying to understand where are the formulas for Spin Orbital Coupling(SOC) term, like Dresselhaus term and Raashba term come from.

- Kane & Mele: generalization to ½-spin electrons, considering SOC

$$H = t\sum_{\langle i,j\rangle} c_i^\dagger c_j + i\lambda_{SO}\sum_{\langle\langle i,j\rangle\rangle} v_{ij} c_i^\dagger s_z c_j + i\lambda_R \sum_{\langle i,j\rangle} c_i^\dagger (\boldsymbol{s}\times\boldsymbol{d}_{ij})_z c_j$$

$$+\lambda_v \sum_i \xi_i c_i^\dagger c_i \qquad where\ c_i^\dagger = (c_{i,\uparrow}^\dagger, c_{i,\downarrow}^\dagger)$$

Graph 1: *Screenshot from Tongyang Zhao's ppt*

For quasi-2D electron gas, the Rashba spin-orbit coupling is induced by structure inversion asymmetry (SIA) (along *z* axis), which can be tuned by gate.

$$H = \frac{\hbar^2 k^2}{2m_{\text{eff}}} + \alpha_{so}\vec{e}_z\cdot(\boldsymbol{k}\times\vec{\sigma}), \qquad \alpha_{so} \propto \langle \nabla_z V(\boldsymbol{r})\rangle \neq 0.$$

The Dresselhaus spin-orbit coupling is due to bulk inversion asymmetry (BIA):

$$H = \frac{\hbar^2 k^2}{2m_{\text{eff}}} + \beta_{so}(k_x\sigma_x - k_y\sigma_y),$$

Graph 2: *Screenshot from Pro.Liu's ppt[3]*

And most of the contents can be found in books([1] and [2]). More specifically, the kp method is illustrated by both the books, the invariant method to construct Hamiltonian is detailed in chapter 5 of book[2], and the example of deriving the Dresselhaus and Rashba term of SOC can is showed in chapter6 of book[1].

The formula of Rashba term in graphene lattice can be found in [4], and the methods to construct matrix basis for off-diagonal block is shown in the Appendix of [5].

II. THE ORIGIN OF SOC

From Relative Quantum Mechanics, we have Dirac equation:

$$\left(c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m_0 c^2 + V\right)\psi = E\psi$$

where

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}$$

$$\beta = \begin{pmatrix} 1_{2\times 2} & 0 \\ 0 & -1_{2\times 2} \end{pmatrix}$$

rewrite the coupled equations for the upper and lower pairs of components, ψ_{A} and ψ_{B}, as follows:

$$\begin{aligned} \sigma \cdot \boldsymbol{p}\psi_{\mathrm{B}} &= \frac{1}{c}(\tilde{E} - V)\psi_{\mathrm{A}} \\ \sigma \cdot p\psi_{\mathrm{A}} &= \frac{1}{c}\left(\tilde{E} - V + 2m_0c^2\right)\psi_{\mathrm{B}} \end{aligned}$$

where $\tilde{E} = E - m_0c^2$. Using the second equation, we can eliminate ψ_{B} in the first equation to obtain:

$$\sigma \cdot p\left[\frac{c^2}{\widetilde{E} - V + 2m_0c^2}\right]\sigma \cdot p\psi_{\mathrm{A}} = (\tilde{E} - V)\psi_{\mathrm{A}}$$

Using approximation:

$$\frac{c^2}{\tilde{E} - V + 2m_0c^2} \approx \frac{1}{2m_0}\left[1 - \frac{\tilde{E} - V}{2m_0c^2} + \dots\right]$$

and replace ψ_{A} by a new two-component wave function:

$$\tilde{\psi} = \left(1 + \frac{p^2 + e\hbar\sigma \cdot B}{8m_0^2c^2}\right)\psi_{\mathrm{A}}$$

Therefore, we have the Pauli equation:

$$\left[\tfrac{p^2}{2m_0} + V + \tfrac{e\hbar}{2m_0}\sigma \cdot B - \tfrac{e\hbar\sigma\cdot p\times\mathcal{E}}{4m_0^2c^2} - \tfrac{e\hbar^2}{8m_0^2c^2}\nabla \cdot \mathcal{E} \right.$$
$$\left. - \tfrac{p^4}{8m_0^3c^2} - \tfrac{e\hbar p^2}{4m_0^3c^2}\sigma \cdot B - \tfrac{(e\hbar B)^2}{8m_0^3c^2}\right]\tilde{\psi} = \tilde{E}\tilde{\psi}$$

where $\mathcal{E} = (1/e)\nabla V$ is the electric field. Normally, we write the Pauli SO term as:

$$H_{\mathrm{SO}} = -\frac{\hbar}{4m_0^2c^2}\sigma \cdot p \times (\nabla V_0)$$

III. SOC IN SOLID SYSTEM

Here, we employ $\boldsymbol{k} \cdot \boldsymbol{p}$ method to study the SOC in Solid State System:

$$\left[\frac{p^2}{2m_0} + V_0(\boldsymbol{r})\right] \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} u_{\nu\boldsymbol{k}}(\boldsymbol{r}) = E_\nu(\boldsymbol{k})\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} u_{\nu\boldsymbol{k}}(\boldsymbol{r}) \tag{1}$$

$$\left[\frac{p^2}{2m_0} + V_0 + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0}\boldsymbol{k}\cdot\boldsymbol{p}\right] |\nu\boldsymbol{k}\rangle = E_\nu(\boldsymbol{k})|\nu\boldsymbol{k}\rangle \tag{2}$$

include SOC term:

$$\begin{aligned}\left[\frac{p^2}{2m_0} + V_0 + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0}k\cdot\pi + \frac{\hbar}{4m_0^2c^2}\boldsymbol{p}\cdot\boldsymbol{\sigma}\times(\nabla V_0)\right]|nk\rangle \\ = E_n(\boldsymbol{k})|nk\rangle\end{aligned} \tag{3}$$

where:

$$\pi := p + \frac{\hbar}{4m_0c^2}\sigma \times \nabla V_0 \tag{4}$$

if we can expand the k state in terms of band edge state, then we can treat the k-dependent terms as small perturbations.

IV. PRE-KNOWLEDGE OF GROUP THEORY

Group

Representation and Basis

Reducible and Irreducible

$$\widehat{\mathrm{P}}_{\mathrm{g}}\widehat{\mathrm{H}}(\overrightarrow{\mathrm{x}}) = \widehat{\mathrm{H}}(\overrightarrow{\mathrm{x}})\widehat{\mathrm{P}}_{\mathrm{g}} \tag{5}$$

$$\widehat{\mathrm{H}}(\overrightarrow{\mathrm{x}})\widehat{\mathrm{P}}_{\mathrm{g}}\Psi_i(\overrightarrow{\mathrm{x}}) = \widehat{\mathrm{P}}_{\mathrm{g}}\widehat{\mathrm{H}}(\overrightarrow{\mathrm{x}})\Psi_i(\overrightarrow{\mathrm{x}}) = \widehat{\mathrm{P}}_{\mathrm{g}}\mathrm{E}_{\mathrm{n}}\Psi_i(\overrightarrow{\mathrm{x}}) = \mathrm{E}_{\mathrm{n}}\widehat{\mathrm{p}}_{\mathrm{g}}\Psi_i(\overrightarrow{\mathrm{x}}) \tag{6}$$

$$\widehat{\mathrm{P}_{\mathrm{g}}}\Psi_i(\overrightarrow{\mathrm{x}}) = \sum_{i'=1}^{l} \Delta^{(\mathrm{n})}_{i'i}(\mathrm{g})\Psi_{i'}(\overrightarrow{\mathrm{x}}) \tag{7}$$

It means the wave functions of the same energy can transform as a representation. Apart from that, we can also prove that the basis of the irreducible representation must have the same energy.

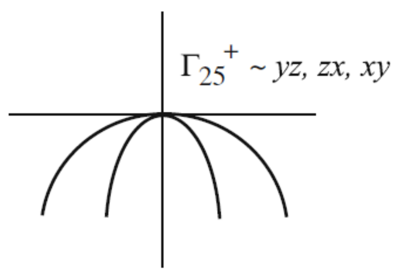

Fig. 3.1 Three-band model for diamond-type semiconductors

Table 3.1 Symmetries of states at the Γ point for diamond structure [5, 24]. The second column gives the orbitals on the two atoms in the basis. The far-right column gives the corresponding plane-wave states

		Cardona and Pollak [5]		
Γ_1^+	$s_a + s'_a$	Γ_1^l	s^+	[000]
Γ_{25}^+	$p_a - p'_a \sim yz, zx, xy$	$\Gamma_{25'}^l$	p^+	[111]
Γ_2^-	$s_a - s'_a \sim xyz$	$\Gamma_{2'}^l$	s^-	[111]
Γ_{15}^-	$p_a + p'_a \sim x, y, z$	Γ_{15}	p^-	[111]
Γ_{12}^-	$d_a - d'_a \sim \sqrt{3}\left(y^2 - z^2\right), 3x^2 - r^2$	$\Gamma_{12'}$	d^-	[200]
Γ_1^+	$s_a + s'_a$	Γ_1^u	s^+	[111]
Γ_{25}^+	$d_a + d'_a \sim yz, zx, xy$	$\Gamma_{25'}^u$	d^+	[200]
Γ_2^-	$s_a - s'_a \sim xyz$	$\Gamma_{2'}^u$	s^-	[200]

Graph 3: *Valence band of DM and Representation of Point Group Oh.[2]*

V. TOOLS IN SOLVING THE SOLID SYSTEM

Then we let's take a look at the original equation again:

$$\begin{aligned}\left[\frac{p^2}{2m_0}+V_0+\frac{\hbar^2k^2}{2m_0}+\frac{\hbar}{m_0}k\cdot\pi+\frac{\hbar}{4m_0^2c^2}\boldsymbol{p}\cdot\boldsymbol{\sigma}\times(\nabla V_0)\right]|nk\rangle \\ =E_n(\boldsymbol{k})|nk\rangle\end{aligned} \tag{8}$$

and we can neglect the SOC term at first, to get some knowledge with the methods we will use.

A. Second Order Perturbation

$$\sim \left\langle \varepsilon_r^+|\mathbf{k}\cdot\mathbf{p}|\varepsilon_s^+\right\rangle = 0 \tag{9}$$

$$\begin{aligned}H_{rs}\equiv\langle r|H(\mathbf{k})|s\rangle &= \frac{\hbar^2}{m_0^2}\sum_{l\alpha v}\frac{\langle r|\mathbf{k}\cdot\mathbf{p}|l\alpha v\rangle\langle l\alpha v|\mathbf{k}\cdot\mathbf{p}|s\rangle}{E_{\Gamma_{25}^+}-E_{l\alpha}} \\ &= \frac{\hbar^2}{m_0^2}k_ik_j\sum_{l\alpha v}{}^{'}\frac{\langle r\left|p_i\right|l\alpha v\rangle\langle l\alpha v\left|p_j\right|s\rangle}{E_{\Gamma_{25}^+}-E_{l\alpha}}\end{aligned} \tag{10}$$

$$H_{33}=\frac{\hbar^2}{m_0^2}\sum_{l\alpha v}{}^{'}\left\{k_z^2\frac{\left|\langle xy\left|p_z\right|l\alpha v\rangle\right|^2}{E_{T_{25}^+}-E_{l\alpha}}+\left(k_x^2+k_y^2\right)\frac{\left|\langle xy\left|p_y\right|l\alpha v\rangle\right|^2}{E_{\Gamma_{25}^+}-E_{l\alpha}}\right\} \tag{11}$$

$$H_{\mathrm{DKK}}(\mathbf{k})=\begin{pmatrix} |yz\rangle & |zx\rangle & |xy\rangle \\ Lk_x^2+M\left(k_y^2+k_z^2\right) & Nk_xk_y & Nk_xk_z \\ Nk_xk_y & Lk_y^2+M\left(k_z^2+k_x^2\right) & Nk_yk_z \\ Nk_xk_z & Nk_yk_z & Lk_z^2+M\left(k_x^2+k_y^2\right)\end{pmatrix} \tag{12}$$

B. Lowdin Perturbation

$$\sum_{n=1}^{N} \left[H_{mn} - E\delta_{mn} \right] C_n = 0, m = 1, N \tag{13}$$

$$\psi = \sum_{m \in A} \psi_m^{(0)} + \sum_{n \in B} \psi_n^{(0)} \tag{14}$$

$$\begin{gathered} \left(E - H_{mm}\right) C_m = \textstyle\sum_{n \in A} H'_{mn} C_n + \sum_{n \in B} H'_{mn} C_n \\ H'_{mn} \equiv H_{mn} \left(1 - \delta_{mn}\right) \end{gathered} \tag{15}$$

$$C_m = \left(\sum_{n \in A} + \sum_{n \in B} \right) \frac{H'_{mn}}{E - H_{mm}} C_n \equiv \left(\sum_{n \in A} + \sum_{n \in B} \right) h'_{mn} C_n \tag{16}$$

$$\begin{aligned} C_m &= \sum_{n \in A} h'_{mn} C_n + \sum_{n \in B} h'_{mn} C_n \\ &= \sum_{n \in A} h'_{mn} C_n + \sum_{n \in B} h'_{mn} \left[\sum_{\alpha \in A} h'_{n\alpha} C_\alpha + \sum_{\alpha \in B} h'_{n\alpha} C_\alpha \right] \\ &= \sum_{n \in A} h'_{mn} C_n + \sum_{n \in A} \sum_{\alpha \in B} h'_{\alpha n} h'_{m\alpha} C_n + \sum_{n \in A} \sum_{\alpha, \beta \in B} h'_{\beta n} h'_{m\alpha} h'_{\alpha\beta} C_n + \cdots \\ &= \sum_{n \in A} h'_{mn} C_n + \sum_{n \in A} \sum_{\alpha \in B} h'_{\alpha n} h'_{m\alpha} C_n + \sum_{n \in A} \sum_{\alpha, \beta \in B} h'_{\beta n} h'_{m\alpha} h'_{\alpha\beta} C_n + \cdots \\ &= \frac{1}{\left(E - H_{mm}\right)} \sum_{n \in A} \left[U^A_{mn} - H_{mn} \delta_{mn} \right] C_n \end{aligned} \tag{17}$$

$$U^A_{mn} \equiv H_{mn} + \sum_{\alpha \in B} \frac{H_{m\alpha} H_{\alpha n}}{\left(E - H_{\alpha\alpha}\right)} + \sum_{\alpha, \beta \in B} \frac{H_{m\alpha} H_{\alpha\beta} H_{\beta n}}{\left(E - H_{\alpha\alpha}\right) \left(E - H_{\beta\beta}\right)} \tag{18}$$

C. Invariant Method

$$\psi'_i(\mathbf{r}) = \psi_i \left(G^{-1} \mathbf{r} \right) = \sum_j \psi_j(\mathbf{r}) D_{ji}(G) \tag{19}$$

$$H'(\mathcal{K}) = D^{-1}(G)H(\mathcal{K})D(G) \tag{20}$$

$$H'(\mathcal{K}') = D(G)H\left(G^{-1}\mathcal{K}\right)D^{-1}(G) = H(\mathcal{K}) \tag{21}$$

$$X_i' = G^{-1}X_i = D(G)X_iD^{-1}(G) = \sum_j X_j D_{ji}^{(X)}(G) \tag{22}$$

$$D_{iji'j'}^{(X)} = D_{ii'}D_{jj'}^{-1} = D_{ii'}D_{jj'}^{*} \tag{23}$$

$D^{(X)}$ is the direct product $D \otimes D^*$

D. Valence Band of Diamond without SOC

$$I_x, I_y, I_z, I_x^2, I_y^2, \{I_xI_y\}, \{I_yI_z\}, \{I_zI_x\} \tag{24}$$

$$\mathbf{k} \sim \Gamma_{15}^-, \mathbf{I} \sim \Gamma_{15}^+ \tag{25}$$

$$\begin{aligned} \Gamma_{15}^- \otimes \Gamma_{15}^- &= \Gamma_1^+ \oplus \Gamma_{12}^+ \oplus \Gamma_{15}^+ \oplus \Gamma_{25}^+ \\ \Gamma_{15}^+ \otimes \Gamma_{15}^+ &= \Gamma_1^+ \oplus \Gamma_{12}^+ \oplus \Gamma_{15}^+ \oplus \Gamma_{25}^+ \end{aligned} \tag{26}$$

Table 5.1 Irreducible basis functions for O_h in 3×3 subspace. $\omega = e^{2\pi i/3}$, $\{AB\} = \frac{1}{2}(AB + BA)$, $[A, B] = (AB - BA)$

	Time reversal	
	Even	Odd
Γ_1^+	k^2, I^2	
Γ_{12}^+	$k_x^2 + \omega k_y^2 + \omega^2 k_z^2, k_x^2 + \omega^2 k_y^2 + \omega k_z^2$ $I_x^2 + \omega I_y^2 + \omega^2 I_z^2, I_x^2 + \omega^2 I_y^2 + \omega I_z^2$	
Γ_{15}^+		I_x, I_y, I_z $[k_y, k_z], [k_z, k_x], [k_x, k_y]$ $\sigma_x, \sigma_y, \sigma_z$
Γ_{25}^+	$\{k_y k_z\}, \{k_z k_x\}, \{k_x k_y\}$ $\{I_y I_z\}, \{I_z I_x\}, \{I_x I_y\}$	
Γ_{15}^-		k_x, k_y, k_z

Graph 4: *From [2]*

$$
\begin{aligned}
H(\mathbf{k}) =& \alpha_1 k^2 + \alpha_2 \left(k_x^2 I_x^2 + k_y^2 I_y^2 + k_z^2 I_z^2\right) \\
& + \alpha_3 \left(\{k_x k_y\}\{I_x I_y\} + \{k_y k_z\}\{I_y I_z\} + \{k_z k_x\}\{I_z I_x\}\right) \\
=& A k^2 - (A - B)\left(k_x^2 I_x^2 + k_y^2 I_y^2 + k_z^2 I_z^2\right) \\
& - 2C \left(\{k_x k_y\}\{I_x I_y\} + \{k_y k_z\}\{I_y I_z\} + \{k_z k_x\}\{I_z I_x\}\right)
\end{aligned} \tag{27}
$$

$$
H(\mathbf{k}) = \begin{pmatrix}
\alpha_1 k^2 + \alpha_2 \left(k_y^2 + k_z^2\right) & -\frac{\alpha_3}{2} k_x k_y & -\frac{\alpha_3}{2} k_x k_z \\
-\frac{\alpha_3}{2} k_x k_y & \alpha_1 k^2 + \alpha_2 \left(k_x^2 + k_z^2\right) & -\frac{\alpha_3}{2} k_y k_z \\
-\frac{\alpha_3}{2} k_x k_z & -\frac{\alpha_3}{2} k_y k_z & \alpha_1 k^2 + \alpha_2 \left(k_x^2 + k_y^2\right)
\end{pmatrix} \tag{28}
$$

E. Valence Band of Diamond With SOC

$$
\begin{aligned}
& 1, J_x, J_y, J_z, J_x^2, J_y^2, \{J_x J_y\}, \{J_y J_z\}, \{J_z J_x\} \\
& \left\{\left(J_y^2 - J_z^2\right) J_x\right\} \equiv V_x, \{(J_z^2 - J_x^2) J_y\} \equiv V_y, \left\{\left(J_x^2 - J_y^2\right) J_z\right\} \equiv V_z \\
& J_x^3, J_y^3, J_z^3, J_x J_y J_z + J_z J_y J_x
\end{aligned} \tag{29}
$$

Table 5.2 Irreducible basis functions, operators, and tensors for O_h' in 4×4 subspace [1]. $\omega = e^{2\pi i/3}$, $\{AB\} = \frac{1}{2}(AB + BA)$

	Time reversal	
	Even	Odd
Γ_1^+	k^2, J^2	
Γ_2^+		$J_x J_y J_z + J_z J_y J_x$
Γ_{12}^+	$k_x^2 + \omega k_y^2 + \omega^2 k_z^2$, $k_x^2 + \omega^2 k_y^2 + \omega k_z^2$	
	$J_x^2 + \omega J_y^2 + \omega^2 J_z^2$, $J_x^2 + \omega^2 J_y^2 + \omega J_z^2$	
Γ_{15}^+		$J_x, J_y, J_z; J_x^3, J_y^3, J_z^3; \sigma_x, \sigma_y, \sigma_z$
		$[k_y, k_z], [k_z, k_x], [k_x, k_y]$
Γ_{25}^+	$\{k_y k_z\}, \{k_z k_x\}, \{k_x k_y\}$	V_x, V_y, V_z
	$\{J_y J_z\}, \{J_z J_x\}, \{J_x J_y\}$	
Γ_{15}^-		k_x, k_y, k_z
Γ_1^-		$k_x\sigma_x + k_y\sigma_y + k_z\sigma_z$
Γ_{12}^-		$K_1 = k_x\sigma_x + \omega k_y\sigma_y + \omega^2 k_z\sigma_z$, $K_2 = K_1^\dagger$
Γ_{25}^-		$k_x\sigma_y + k_y\sigma_x, k_y\sigma_z + k_z\sigma_y, k_x\sigma_z + k_z\sigma_x$

Graph 5: *From [2]*

VI. BIA AND SIA

A. Dresselhaus Term(BIA)

Dresselhaus Term in 3D system is as below(to third order in k), which can be easily shown by the tables below.

$$\mathcal{H}_{6c6c}^{b} = \mathrm{b}_{41}^{6c6c} \begin{pmatrix} \frac{1}{2}\left\{k_+^2 + k_-^2, k_z\right\} & \frac{1}{4}\left\{k_+^2 - k_-^2, k_-\right\} - \left\{k_z^2, k_+\right\} \\ \frac{1}{4}\left\{k_-^2 - k_+^2, k_+\right\} - \left\{k_z^2, k_-\right\} & \end{pmatrix} \tag{30}$$

For 2D quantum well system, we can replace kz term by expectation value $\langle(-i\partial_z)^n\rangle$, and then if we only include the linear in k term, we will get the standard 2D Dresselhaus

SOC Term:

$$\mathcal{H}^{b}_{6c6c} = \mathrm{b}^{6c66}_{41} \begin{pmatrix} 0 & \frac{1}{4}k_{-}\left(k_{+}^{2} - k_{-}^{2}\right) - k_{+}\left\langle k_{z}^{2}\right\rangle \\ \frac{1}{4}k_{+}\left(k_{-}^{2} - k_{+}^{2}\right) - k_{-}\left\langle k_{z}^{2}\right\rangle & 0 \end{pmatrix} \tag{31}$$

Table 5.11 Symmetrized matrices for 14-band model of zincblende. $\{AB\} = \frac{1}{2}(AB + BA)$

Block	Representations	Symmetrized matrices	Time reversal
H^{66}	$\Gamma_6 \otimes \Gamma_6^* = \Gamma_1 \oplus \Gamma_{25}$	$\Gamma_1 : 1_\sigma$	$+$
		$\Gamma_{25} : \sigma_x, \sigma_y, \sigma_z$	$-$
H^{88}	$\Gamma_8 \otimes \Gamma_8^*$		
	$= \Gamma_1 \oplus \Gamma_2 \oplus \Gamma_{12}$	$\Gamma_1 : 1_{4\times4}, J^2$	$+$
	$\oplus 2\Gamma_{15} \oplus 2\Gamma_{25}$	$\Gamma_2 : J_x J_y J_z + J_z J_y J_z$	$-$
		$\Gamma_{12} : \sqrt{3}(J_z^2 - \frac{1}{3}J^2), J_x^2 - J_y^2$	$+$
		$\Gamma_{15} : \{J_x J_y\}, \{J_y J_z\}, \{J_z J_x\};$	$+$
		$\{(J_y^2 - J_z^2)J_x\}, \{(J_z^2 - J_x^2)J_y\}, \{(J_x^2 - J_y^2)J_z\}$	$-$
		$\Gamma_{25} : J_x, J_y, J_z; J_x^3, J_y^3, J_z^3$	$-$
H^{77}	$\Gamma_7 \otimes \Gamma_7^* = \Gamma_1 \oplus \Gamma_{25}$	$\Gamma_1 : 1_\sigma$	$+$
		$\Gamma_{25} : \sigma_x, \sigma_y, \sigma_z$	$-$
H^{68}	$\Gamma_6 \otimes \Gamma_8^*$	$\Gamma_{12} : T_{xx} - T_{yy}, -\sqrt{3}T_{zz}$	
	$= \Gamma_{12} \oplus \Gamma_{15} \oplus \Gamma_{25}$	$\Gamma_{15} : T_x, T_y, T_z$	
		$\Gamma_{25} : T_{yz}, T_{zx}, T_{xy}$	
H^{67}	$\Gamma_6 \otimes \Gamma_7^* = \Gamma_2 \oplus \Gamma_{15}$	$\Gamma_1 : 1_\sigma$	
		$\Gamma_{15} : \rho_x, \rho_y, \rho_z$	
H^{87}	$\Gamma_8 \otimes \Gamma_7^*$	$\Gamma_{12} : \sqrt{3}U_{zz}, U_{xx} - U_{yy},$	
	$= \Gamma_{12} \oplus \Gamma_{15} \oplus \Gamma_{25}$	$\Gamma_{15} : U_{yz}, U_{zx}, U_{xy}$	
		$\Gamma_{25} : U_x, U_y, U_z$	

Graph 6

Table 5.12 Irreducible tensors for 14-band model of zincblende. They are separated into time-reversal even and odd combinations. $\{AB\} = \frac{1}{2}(AB + BA)$

		Time reversal
Terms from wave vector:		
Γ_1	$1, k^2$	$+$
Γ_{12}	$\sqrt{3}\left(k_z^2 - \frac{1}{3}k^2\right), k_x^2 - k_y^2$	$+$
Γ_{15}	$\{k_x k_y\}, \{k_y k_z\}, \{k_z k_x\}$	$+$
	k_x, k_y, k_z	$-$
Terms from magnetic field:		
Γ_1	B^2	$+$
Γ_{12}	B_x^2, B_y^2	$+$
Γ_{15}	$B_x B_y, B_y B_z, B_z B_x$	$+$
Γ_{25}	B_x, B_y, B_z	$-$
Terms from strain interaction:		
Γ_1	$\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$	$+$
Γ_{12}	$\sqrt{3}\left(\varepsilon_{zz} - \frac{1}{3}\mathrm{Tr}\varepsilon\right), \varepsilon_{xx} - \varepsilon_{yy}$	$+$
Γ_{15}	$\varepsilon_{yz}, \varepsilon_{zx}, \varepsilon_{xy}$	$+$
Mixed terms:		
Γ_1	$k_x\varepsilon_{yz} + k_y\varepsilon_{zx} + k_z\varepsilon_{xy}$	$-$
Γ_{12}	$\frac{1}{\sqrt{3}}\left(2k_z\varepsilon_{xy} - k_x\varepsilon_{yz} - k_y\varepsilon_{zx}\right), \left(k_x\varepsilon_{yz} - k_y\varepsilon_{zx}\right)$	$-$
Γ_{15}	$k_y\varepsilon_{xy} + k_z\varepsilon_{xz}, k_z\varepsilon_{yz} + k_x\varepsilon_{yx}, k_x\varepsilon_{zx} + k_y\varepsilon_{zy};$	$-$
	$k_x\left(\varepsilon_{xx} - \frac{1}{3}\mathrm{Tr}\varepsilon\right), k_y\left(\varepsilon_{yy} - \frac{1}{3}\mathrm{Tr}\varepsilon\right), k_z\left(\varepsilon_{zz} - \frac{1}{3}\mathrm{Tr}\varepsilon\right);$	$-$
	$k_x\mathrm{Tr}\varepsilon, k_y\mathrm{Tr}\varepsilon, k_z\mathrm{Tr}\varepsilon$	$-$
Γ_{25}	$\left(k_y\varepsilon_{xy} - k_z\varepsilon_{xz}\right), \left(k_z\varepsilon_{yz} - k_x\varepsilon_{yx}\right), \left(k_x\varepsilon_{zx} - k_y\varepsilon_{zy}\right);$	$-$
	$k_x\left(\varepsilon_{yy} - \varepsilon_{zz}\right), k_y\left(\varepsilon_{zz} - \varepsilon_{xx}\right), k_z\left(\varepsilon_{xx} - \varepsilon_{yy}\right)$	$-$

Graph 7

B. Rashba Term(SIA)

If we include macroscopic field which breaks the inversion symmetry, we will see structure inversion asymmetry induced spin splitting, which is expressed by the Rashba SOC term:

$$\mathcal{H}^{r}_{6c6c} = r^{6c6c}_{41}\sigma \cdot k \times \mathcal{E} \tag{32}$$

This is also simple, since this is the only invariant term allowed, to the first order in k.

Table C.3. (a) Symmetrized matrices for the matrix expansion of the blocks $\mathcal{H}_{\alpha\beta}$ for the point group T_d [2]. The matrices σ_i, J_i, T_i, and U_i are given in Table C.2. For the diagonal blocks, we also give the symmetry with respect to time reversal. Notation: $\{A,B\} = \frac{1}{2}(AB + BA)$

Block	Representations		Symmetrized matrices	Time reversal
$\mathcal{H}_{66}$	$\Gamma_6 \times \Gamma_6^*$	Γ_1 :	$\mathbb{1}_{2\times 2}$	+
	$= \Gamma_1 + \Gamma_4$	Γ_4 :	$\sigma_x, \sigma_y, \sigma_z$	−
$\mathcal{H}_{77}$	$\Gamma_7 \times \Gamma_7^*$	Γ_1 :	$\mathbb{1}_{2\times 2}$	+
	$= \Gamma_1 + \Gamma_4$	Γ_4 :	$\sigma_x, \sigma_y, \sigma_z$	−
$\mathcal{H}_{88}$	$\Gamma_8 \times \Gamma_8^*$	Γ_1 :	$\mathbb{1}_{4\times 4}$; J^2	+
	$= \Gamma_1 + \Gamma_2 + \Gamma_3$	Γ_2 :	$J_x J_y J_z + J_z J_y J_x$	−
	$+2\Gamma_4 + 2\Gamma_5$	Γ_3 :	$\frac{1}{\sqrt{3}}(2J_z^2 - J_x^2 - J_y^2), J_x^2 - J_y^2$	+
		Γ_4 :	J_x, J_y, J_z;	−
			J_x^3, J_y^3, J_z^3	−
		Γ_5 :	$\{J_y, J_z\}, \{J_z, J_x\}, \{J_x, J_y\}$;	+
			$\{J_x, J_y^2 - J_z^2\}, \{J_y, J_z^2 - J_x^2\},$ $\{J_z, J_x^2 - J_y^2\}$	−
$\mathcal{H}_{67}$	$\Gamma_6 \times \Gamma_7^*$	Γ_2 :	$\mathbb{1}_{2\times 2}$	
	$= \Gamma_2 + \Gamma_5$	Γ_5 :	$\sigma_x, \sigma_y, \sigma_z$	
$\mathcal{H}_{68}$	$\Gamma_6 \times \Gamma_8^*$	Γ_3 :	$T_{xx} - T_{yy}, -\sqrt{3}T_{zz}$	
	$= \Gamma_3 + \Gamma_4 + \Gamma_5$	Γ_4 :	T_{yz}, T_{zx}, T_{xy}	
		Γ_5 :	T_x, T_y, T_z	
$\mathcal{H}_{87}$	$\Gamma_8 \times \Gamma_7^*$	Γ_3 :	$\sqrt{3}U_{zz}, U_{xx} - U_{yy}$,	
	$= \Gamma_3 + \Gamma_4 + \Gamma_5$	Γ_4 :	U_x, U_y, U_z	
		Γ_5 :	U_{yz}, U_{zx}, U_{xy}	

Graph 8

Table C.4. Irreducible tensor components for the point group T_d. Notation: $\{\ldots\}$ denotes the symmetrized product of its arguments, e.g. $\{A, B\} = \frac{1}{2}(AB + BA)$

Γ_1	$1;\quad k^2;\quad \{k_x, k_y, k_z\};\quad k^4;\quad \{k_x, k_y\}^2 + \{k_y, k_z\}^2 + \{k_z, k_x\}^2;\quad -B^2;$ $V;\quad \boldsymbol{\mathcal{E}} \cdot \boldsymbol{k};\quad \mathcal{E}_x\{k_y, k_z\} + \mathcal{E}_y\{k_z, k_x\} + \mathcal{E}_z\{k_x, k_y\};\quad \nabla \cdot \boldsymbol{\mathcal{E}}$
Γ_2	$\boldsymbol{B} \cdot \boldsymbol{k};\quad B_x\{k_y, k_z\} + B_y\{k_z, k_x\} + B_z\{k_x, k_y\};\quad \boldsymbol{\mathcal{E}} \cdot \boldsymbol{B}$
Γ_3	$\frac{1}{\sqrt{3}}(2k_z^2 - k_x^2 - k_y^2), k_x^2 - k_y^2;\quad \frac{1}{\sqrt{3}}(2k_z^4 - k_x^4 - k_y^4), k_x^4 - k_y^4;$ $\frac{1}{\sqrt{3}}(2\{k_x^2, k_y^2\} - \{k_y^2, k_z^2\} - \{k_z^2, k_x^2\}), \{k_y^2, k_z^2\} - \{k_z^2, k_x^2\};$ $B_x k_x - B_y k_y, \frac{1}{\sqrt{3}}(-2B_z k_z + B_x k_x + B_y k_y);$ $B_x\{k_y, k_z\} - B_y\{k_z, k_x\}, \frac{1}{\sqrt{3}}(-2B_z\{k_x, k_y\} + B_x\{k_y, k_z\} + B_y\{k_z, k_x\});$ $\frac{1}{\sqrt{3}}(2B_z^2 - B_x^2 - B_y^2), B_x^2 - B_y^2;\quad \frac{1}{\sqrt{3}}(2\mathcal{E}_z k_z - \mathcal{E}_x k_x - \mathcal{E}_y k_y), \mathcal{E}_x k_x - \mathcal{E}_y k_y;$ $\frac{1}{\sqrt{3}}(2\mathcal{E}_z\{k_x, k_y\} - \mathcal{E}_x\{k_y, k_z\} - \mathcal{E}_y\{k_z, k_x\}), \mathcal{E}_x\{k_y, k_z\} - \mathcal{E}_y\{k_z, k_x\};$ $\mathcal{E}_x B_x - \mathcal{E}_y B_y, \frac{1}{\sqrt{3}}(-2\mathcal{E}_z B_z + \mathcal{E}_x B_x + \mathcal{E}_y B_y)$
Γ_4	$\{k_x, k_y^2 - k_z^2\}, \{k_y, k_z^2 - k_x^2\}, \{k_z, k_x^2 - k_y^2\};$ $\{k_y^3, k_z\} - \{k_y, k_z^3\}, \{k_z^3, k_x\} - \{k_z, k_x^3\}, \{k_x^3, k_y\} - \{k_x, k_y^3\};$ $B_x, B_y, B_z;\quad B_y k_z + B_z k_y, B_z k_x + B_x k_z, B_x k_y + B_y k_x;$ $k^2 B_x, k^2 B_y, k^2 B_z;\quad k_x^2 B_x, k_y^2 B_y, k_z^2 B_z;$ $\{k_x, k_y\}B_y + \{k_x, k_z\}B_z, \{k_y, k_z\}B_z + \{k_y, k_x\}B_x, \{k_z, k_x\}B_x + \{k_z, k_y\}B_y;$ $\mathcal{E}_z k_y - \mathcal{E}_y k_z, \mathcal{E}_x k_z - \mathcal{E}_z k_x, \mathcal{E}_y k_x - \mathcal{E}_x k_y;$ $\mathcal{E}_x\{k_y^2 - k_z^2\}, \mathcal{E}_y\{k_z^2 - k_x^2\}, \mathcal{E}_z\{k_x^2 - k_y^2\};$ $\mathcal{E}_y\{k_x, k_y\} - \mathcal{E}_z\{k_x, k_z\}, \mathcal{E}_z\{k_y, k_z\} - \mathcal{E}_x\{k_y, k_x\}, \mathcal{E}_x\{k_z, k_x\} - \mathcal{E}_y\{k_z, k_y\};$ $\mathcal{E}_y B_z + \mathcal{E}_z B_y, \mathcal{E}_z B_x + \mathcal{E}_x B_z, \mathcal{E}_x B_y + \mathcal{E}_y B_x$

Graph 9

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