Construct $\vec{k}\cdot\hat{P}$ Models for Semiconductors

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1, Quick Review of Symmetries in QM

1.1 Symmetry Groups of Crystals

$\hat{H} = \sum_k \hat{c}_k^\dagger\, h(k)\, \hat{c}_k$
$\hat{S}\,\hat{H}\,\hat{S}^{-1} = \hat{H} \to S\,h(\vec{k})\,S^{-1} = h\left(S\,\vec{k}\right),\ S = [\hat{S}]_\psi$
$G_{\vec{k}} = \left\{g \in G \mid g\,h(\vec{k})\,g^{-1} = h\left(g\,\vec{k}\right)\right\}$ → Little group at $\vec{k}$ point, an invariant subgroup of the space group G

8 independent symmorphic operators:
$1,\ 2,\ 3,\ 4,\ 6,\ \overline{4},\ \overline{i},\ m$
$\overline{4} = \overline{i}\,C_4,\ m_{[u,v,w]} = \overline{i}\,C_{2,[u,v,w]} \Rightarrow \hat{C}_{n,\hat{r}} = e^{-\overline{i}\frac{2\pi}{n}\hat{J}\cdot\hat{r}},\ \overline{i},\ \hat{T}\ (n = 1,\ 2,\ 3,\ 4,\ 6)$

1.2 Atomic Orbitals

1.2.1 spinless orbitals: s, $p_{x,y,z}$, E_g, T_{2g}, $\cdots$

$\psi = (\psi_1,\ \psi_2,\ \cdots,\ \psi_N)^T,\ \psi_i = Y_{l_i m_i};$

$$g_i \begin{array}{|c|}\hline \psi_1 \\ \hline \psi_2 \\ \hline \vdots \\ \hline \psi_N \\ \hline\end{array} = \begin{array}{|c|}\hline \psi_1{}' \\ \hline \psi_2{}' \\ \hline \vdots \\ \hline \psi_N{}' \\ \hline\end{array} = M_{N\times N} \begin{array}{|c|}\hline \psi_1 \\ \hline \psi_2 \\ \hline \vdots \\ \hline \psi_N \\ \hline\end{array} \Rightarrow [g_i]_\psi = M_{N\times N};$$

$\hat{T} = K;$

1.2.2 SOC included: $|\,j,\ m\rangle,\ |\,j_1,\ m_1;\ \frac{1}{2},\ \pm\frac{1}{2}\rangle$

$(J_{+,z})_{\alpha\beta} = \langle j_\alpha,\ m_\alpha \mid \hat{J}_{+,z} \mid j_\beta,\ m_\beta\rangle,\ J_- = (J_+)^\dagger$
$\hat{J}_+ \mid j,\ m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\ \left|\,j,\ m+1\right\rangle (m + 1 \leq j)$

$$\hat{C}_{n,[u\,v\,w]} = e^{-\overline{i}\,\frac{2\pi}{n\sqrt{u^2+v^2+w^2}}(u\,J_x + v\,J_y + w\,J_z)} = e^{-\overline{i}\,\frac{2\pi}{n\sqrt{u^2+v^2+w^2}}\left[\frac{u}{2}(J_+ + J_-) + \frac{v}{2\overline{i}}(J_+ - J_-) + w\,J_z\right]}$$
$\hat{T} = e^{-\overline{i}\pi\hat{J}_y}\,K$

refs：

[illegible]Ch-2.8;
C. Cohen-Tannoudji, Quantum Mechanics, Ch-6;
Bernevig, Topological Insulators and Topological Superconductors, Ch-4.

1.3 $k \cdot p$ perturbation term

$$\left(\frac{\hat{p}^2}{2m} + V(\vec{r}) + \frac{\hbar}{4m^2c^2}(\vec{\sigma}\times\nabla V)\cdot\hat{p}\right)\psi_{n,\vec{k}}(\vec{r}) = E_{n,\vec{k}}\,\psi_{n,\vec{k}}(\vec{r})$$

$$\xrightarrow{\psi_{n,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u_{n,\vec{k}}(\vec{r})}\left[\hat{H}_{\vec{k}_0} + \hat{H}_{\mathrm{kp}}\right]u_{n,\vec{k}_0+\vec{k}}(\vec{r}) = \left(E_{n,\vec{k}_0+\vec{k}} - \frac{\hbar^2\left(\vec{k}_0+\vec{k}\right)^2}{2m}\right)u_{n,\vec{k}_0+\vec{k}}(\vec{r})$$

where $\hat{H}_{\mathrm{kp}} = \frac{\hbar}{m}\vec{k}\cdot\hat{P} = \frac{\hbar}{2m}\left(k_+\hat{P}_- + k_-\hat{P}_+\right) + \frac{\hbar}{m}k_z\hat{P}_z$, where $\hat{P} = \hat{p} + \frac{\hbar}{4m^2c^2}(\sigma\times\nabla V)$

$$H = \begin{array}{|c|c|c|c|}\hline \epsilon_{1,\hat{k}_0} & 0 & 0 & 0 \\ \hline 0 & \epsilon_{2,\hat{k}_0} & 0 & 0 \\ \hline 0 & 0 & \ddots & 0 \\ \hline 0 & 0 & 0 & \epsilon_{N,\hat{k}_0} \\ \hline \end{array} + [\hat{H}_{\mathrm{kp},\vec{k}_0}]_\psi;$$

Our task: $[\hat{H}_{\mathrm{kp},\vec{k}_0}]_\psi$ satisfying the symmetry group $G_{\vec{k}_0}$

refs:
[illegible]Ch-3.2;
R. Yu et al, New J. Phys. 17(2015) 023012, Model Hamiltonian for topological Kondo insulator SmB_6.

1.4, Some Properties of Point Groups: Irreps & Character Tables

问题在于, 哈密顿的本征子空间到底荷载着其对称性群的不可约表示呢, 还是也可以荷载可约表示?经过大量研究, 人们相信下面的结论:

系统哈密顿属于任一本征值的本征子空间, 都荷载着其对称性群的一个不可约表示.

这一条规律不能从我们的五条基本原理推出, 也无法给出一般性的证明, 然而人们倾向于认定这是一条普遍的规律. 但是, 当哈密顿具有时间反演对称性时, 这个说法要作适当的补充(见后).

Character Table of the group $D_2(222)$*

$D_2(222)$	#	1	2_z	2_y	2_x	functions
A	Γ_1	1	1	1	1	x^2,y^2,z^2
B_1	Γ_3	1	1	-1	-1	z,xy,J_z
B_2	Γ_2	1	-1	1	-1	y,xz,J_y
B_3	Γ_4	1	-1	-1	1	x,yz,J_x

Table of characters

(1)	(2)	(3)	C_1	C_2	C_3	C_4	C_5
GM_1	A_1	GM_1	1	1	1	1	1
GM_3	B_1	GM_2	1	1	-1	-1	1
GM_4	B_3	GM_3	1	-1	-1	1	1
GM_2	B_2	GM_4	1	-1	1	-1	1
GM_5	$\bar{E}$	$\overline{GM}_5$	2	0	0	0	-2

C_1: 1
C_2: 2_{001}, ${}^d2_{001}$
C_3: 2_{010}, ${}^d2_{010}$
C_4: 2_{100}, ${}^d2_{100}$
C_5: ${}^d1$

Mulliken Symbols for Irreducible Representations

(R. S. Mulliken, *J. Chem. Phys.*, **1955**, *23*, 1997; **1956**, *24*, 1118)

Symbol	Property
A	symmetric with respect to rotation around the principal rotational axis (one dimensional representations)
B	anti-symmetric with respect to rotation around the principal rotational axis (one dimensional representations)
E	degenerate (German: entartet; two dimensional representations, e.g. in systems with higher order principal axes)
subscript 1	symmetric with respect to a vertical mirror plane perpendicular to the principal axis
subscript 2	anti-symmetric with respect to a vertical mirror plane perpendicular to the principal axis
subscript g	symmetric with respect to a center of symmetry (German: "gerade")
subscript u	anti-symmetric with respect to a center of symmetry (German: "ungerade")
prime (')	symmetric with respect to a mirror plane horizontal to the principal rotational axis
double prime ('')	anti-symmetric with respect to a mirror plane horizontal to the principal rotational axis

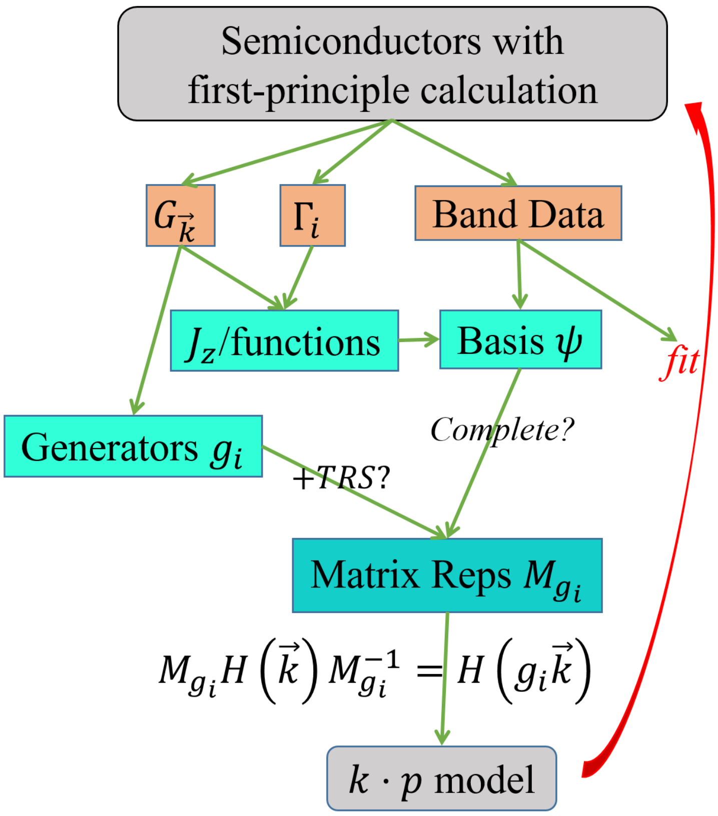
refs :

□□□□□□□□□□□p262;

□□□□□□□□□□□□□□□□□□ch - 2 □□□□□;

Bilbao : http : // www.cryst.ehu.es/

1.5, Step-by-step Overview



1.5, FAQs

Q1, What if minimum orbitals are hard to be grouped as a ECOC?

Quasi-degenerate perturbation theory

refs:
Roland Walker, Spin–Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems, Appendix B;
CC Liu et al, PRB 84, 195430(2011), Low-energy effective Hamiltonian involving spin-orbit coupling in silicene and two-dimensional germanium and tin.

Q2, How to estimate the influence of the SOC term?

Q2.1 SOC of atomic orbitals (spherical symmetry)

$$H_{so} = \xi(r)\,\hat{L}\cdot\hat{S} = \xi(r)\left[\frac{1}{2}\left(\hat{L}_-\hat{S}_+ + \hat{L}_+\hat{S}_-\right) + \hat{S}_z\hat{L}_z\right] = \xi(r)\begin{array}{|c|c|}\hline \hat{L}_z & \frac{1}{2}\hat{L}_+ \\ \hline \frac{1}{2}\hat{L}_- & -\hat{L}_z \\ \hline\end{array};\ (^*\ \Psi = (\psi_\uparrow,\ \psi_\downarrow)^T\ ^*)$$

refs:
M.D. Jones and R.C. Albers, PRB 79, 045107(2009), Spin-orbit coupling in an f-electron tight-binding model: Electronic properties of Th, U, and Pu

Q2.2 Rashba SOC, Dresselhaus SOC

$H_{D_3}{}^{(\Gamma)} = (\gamma/\hbar)[(p_y{}^2 - p_z{}^2)\, p_x\, \sigma_x + c.p.]$

(* zinc-blende III-V semiconductor compounds lacking a centre of inversion *)

$H_R = (\alpha_R/\hbar)\left(\vec{z} \times \hat{p}\right)\cdot\vec{\sigma}$

(* In quantum well with structural inversion broken along $\vec{z}$-direction, resulted by interfacial $\vec{E}$ *)

refs:

A. Manchon et al, Nat. Materials 14, 871(2015), New perspectives for Rashba spin-orbit coupling;

C.L. Kane and E.J. Mele, PRL 95, 226801(2005), Quantum Spin Hall Effect in Graphene;

M.S. Dresselhaus, Springer(2008), Group Theory: Application to the Physics of Condensed Matter, Ch 14.

Q2.3 From definition of SOC term

$H_{so} = \frac{\hbar}{4\, m_0{}^2\, c^2}\left(\nabla V \times \vec{p}\right)\cdot\vec{\sigma} = -\frac{\hbar}{4\, m_0{}^2\, c^2}\left(\vec{F} \times \vec{p}\right)\cdot\vec{\sigma}$

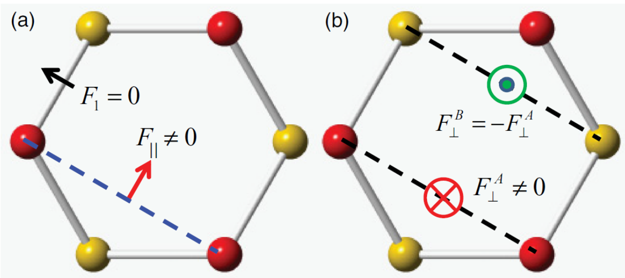


FIG. 2. (Color online) The atomic intrinsic spin-orbit interaction from symmetry considerations. (a) The nearest-neighbor force $F_\perp$ vanishes, while the next-nearest-neighbor force $\vec{F}_{||}$ is nonzero in the horizontal plane. (b) The next-nearest-neighbor nonzero force $F_\perp^A$ equals negative $F_\perp^B$ in the perpendicular direction.

refs:

C.C. Liu et al, PRB 84, 195430(2011), Low-energy effective Hamiltonian involving spin-orbit coupling in silicene and two-dimensional germanium and tin;

R. Yu et al, PRL 119, 036401(2017), From Nodal Chain Semimetal to Weyl Semimetal in HfC, Supplemental Materials

Q3, What if the $\vec{k}$ points is at the boundary of BZ?

We have to find the reps of Space Groups.

Example 1: $D_{4h} + s\, p_{xyz}$ (Cd_3As_2)

1.0 Basis & Reps of Generators

rs of the 3D Crystallographic Point Group D_{4h}(4/mmm)

Show the general positions

Click here to get more detailed information about this point group

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 0,0,z	2_{001}
2	-y,x,z	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	4^{+} 0,0,z	4^{+}_{001}
3	-x,y,-z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	2 0,y,0	2_{010}
4	-x,-y,-z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	-1 0,0,0	-1

C_{2z} conserve the secondary angular momentum up to 2;

$$g_2 \begin{pmatrix} s \\ p_+ \\ p_- \\ p_z \end{pmatrix} = g_2 \begin{pmatrix} s \\ -p_x - i p_y \\ p_x - i p_y \\ p_z \end{pmatrix} = \begin{pmatrix} s \\ p_y - i p_x \\ -p_y - i p_x \\ p_z \end{pmatrix} = \begin{pmatrix} s \\ i p_+ \\ -i p_- \\ p_z \end{pmatrix} \Rightarrow C_{4z} = g_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix};$$

$$g_3 \begin{pmatrix} s \\ p_+ \\ p_- \\ p_z \end{pmatrix} = g_3 \begin{pmatrix} s \\ -p_x - i p_y \\ p_x - i p_y \\ p_z \end{pmatrix} = \begin{pmatrix} s \\ p_x - i p_y \\ -p_x - i p_y \\ -p_z \end{pmatrix} = \begin{pmatrix} s \\ p_- \\ p_+ \\ -p_z \end{pmatrix} \Rightarrow C_{2y} = g_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix};$$

$$P = g_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix};$$

1.1 Write the initial k.p model and Input all reps

```
Clear["Global`*"];
(*basis: S, P+, P-, Pz*)

es = e10 + e11 kp km + e12 kz kz + e13 km km + e13s kp kp;
ex = e20 + e21 kp km + e22 kz kz + e23 km km + e23s kp kp;
ey = e30 + e31 kp km + e32 kz kz + e33 km km + e33s kp kp;
ez = e40 + e41 kp km + e42 kz kz + e43 km km + e43s kp kp;
```

H1= $\begin{pmatrix} \text{es} & \text{a121 kp+a122 km} & \text{a131 kp+a132 km} & \text{a140+a141 kz} \\ \text{a121s km+a122s kp} & \text{ex} & \text{a230+a231 kz} & \text{a241 kp+a242 km} \\ \text{a131s km+a132s kp} & \text{a230s+a231s kz} & \text{ey} & \text{a341 kp+a342 km} \\ \text{a140s+a141s kz} & \text{a241s km+a242s kp} & \text{a341s km+a342s kp} & \text{ez} \end{pmatrix}$;

H2= $\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \text{b233 km}^2\text{+b232 kp}^2 & \text{b241 kp kz} \\ 0 & \text{b232 km}^2\text{+b233 kp}^2 & 0 & \text{-b241 km kz} \\ 0 & \text{b241 km kz} & \text{-b241 kp kz} & 0 \end{pmatrix}$;

C4z= $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$; C2y= $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$; P= $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$;

1.2 k.p models Constrained by symmetries one by one

1.2.1 TRS $(-k_x, -k_y, -k_z)$

```
H1t=FullSimplify[(H1/.{kp→-kp,km→-km,kz→-kz})-Transpose[H1]];
MatrixForm[H1t]
```

$$\begin{pmatrix} 0 & -(\text{a121s}+\text{a122})\ \text{km}-(\text{a121}+\text{a122s})\ \text{kp} & -(\text{a131s}+\text{a132}) \\ -(\text{a121s}+\text{a122})\ \text{km}-(\text{a121}+\text{a122s})\ \text{kp} & 0 & \text{a230}-\text{a230s} \\ -(\text{a131s}+\text{a132})\ \text{km}-(\text{a131}+\text{a132s})\ \text{kp} & -\text{a230}+\text{a230s}-(\text{a231}+\text{a231s})\ \text{kz} & \\ -\text{a140}+\text{a140s}-(\text{a141}+\text{a141s})\ \text{kz} & -(\text{a241s}+\text{a242})\ \text{km}-(\text{a241}+\text{a242s})\ \text{kp} & -(\text{a341s}+\text{a342}) \end{pmatrix}$$

```
a121s=-a122;a122s=-a121;a131s=-a132;a132s=-a131;a140s=a140;a141s=-a141;
a230s=a230;a231s=-a231;a241s=-a242;a242s=-a241;a341s=-a342;a342s=-a341;

MatrixForm[H1t]
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

1.2.2 Inversion $(-k_x, -k_y, -k_z)$

```
Hp=FullSimplify[(H1/.{kp→-kp,km→-km,kz→-kz})-P.H1.Inverse[P]];
MatrixForm[Hp]
```

$$\begin{pmatrix} 0 & 0 & 0 & 2\ \text{a140} \\ 0 & 0 & -2\ \text{a231 kz} & -2\ (\text{a242 km}+\text{a241 kp}) \\ 0 & 2\ \text{a231 kz} & 0 & -2\ (\text{a342 km}+\text{a341 kp}) \\ 2\ \text{a140} & 2\ (\text{a242 km}+\text{a241 kp}) & 2\ (\text{a342 km}+\text{a341 kp}) & 0 \end{pmatrix}$$

```
a140=0;a231=0;a241=0;a242=0;a341=0;a342=0;

MatrixForm[Hp]
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

1.2.3 C2y $(-k_x, k_y, -k_z)$

```
H2y=FullSimplify[(H1/.{kp→-km,km→-kp,kz→-kz})-C2y.H1.Inverse[C2y]];
MatrixForm[H2y]
```

$$\begin{pmatrix} -(e13-e13s)\ (km-kp)\ (km+kp) & -(a121+a132)\ km-(a122+a131)\ kp \\ (a121+a132)\ km+(a122+a131)\ kp & e20-e30+(e23s-e33)\ km^2+(e21-e31)\ km\,kp+(e23-e33s \\ (a122+a131)\ km+(a121+a132)\ kp & 0 \\ 0 & 0 \end{pmatrix}$$

```
e13s=e13;e30=e20;e31=e21;e33s=e23;e32=e22;e23s=e33;e43s=e43;
a132=-a121;a131=-a122;

MatrixForm[H2y]
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

1.2.4 C4z $(-k_y, k_x, k_z)$

```
H4z=FullSimplify[MatrixForm[(H1/.{kp→i kp,km→-i km,kz→kz})-C4z.H1.Inverse[C4z]]];
MatrixForm[H4z]
```

$$\begin{pmatrix} -2\ e13\ (km^2+kp^2) & 2\ i\ a121\ kp & 2\ i\ a121\ km & 0 \\ 2\ i\ a122\ km & -2\ (e23\ km^2+e33\ kp^2) & 2\ a230 & 0 \\ 2\ i\ a122\ kp & 2\ a230 & -2\ (e33\ km^2+e23\ kp^2) & 0 \\ 0 & 0 & 0 & -2\ e43\ (km^2+kp^2) \end{pmatrix}$$

```
e13=0;e23=0;e33=0;e43=0;
a121=0;a230=0;a122=0;

MatrixForm[H4z]
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

1.2.5 Final result

```
kp=kx+ⅈ ky;
km=kx-ⅈ ky;

U= | 1 | 0        | 0         | 0 |
   | 0 | -(√2)/2  | -ⅈ(√2)/2  | 0 |
   | 0 | (√2)/2   | -ⅈ(√2)/2  | 0 |
   | 0 | 0        | 0         | 1 | ;

(* Transform Basis from (s p₊ p₋ p_z) to (s p_x p_y p_z)*)

H_sxyz=Simplify[Inverse[U].H1.U];
MatrixForm[Collect[H_sxyz,{kx,ky,kz}]]
```

$$\left(\begin{array}{ll} e10+(e11+2\,e13)\,kx^2+(e11-2\,e13)\,ky^2+e12\,kz^2 & -\sqrt{2}\,(a121+a122)\,kx \\ \sqrt{2}\,(a121+a122)\,kx & -a230+e20+(e21+e23+e33)\,kx^2+(e21-e\!: \\ \sqrt{2}\,(a121-a122)\,ky & 2\,(-e23+e33)\,kx\,ky \\ -a141\,kz & 0 \end{array}\right.$$

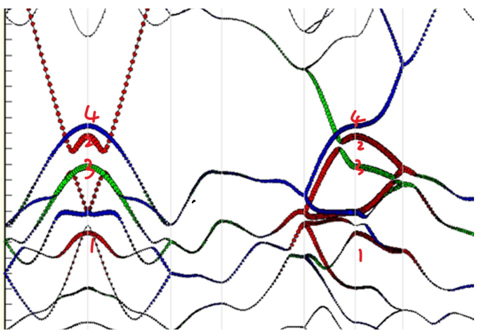
1.3 Check the bands along some high-symmetry paths

Example 2: D2 + $s\,p_{xyz}$ (Ag_2S)

0. Band Infos and Irreducible Reps

0.1 Pick dominant atomic orbitals satisfying symmetries' constrains

(bands without spin-orbit coupling)



Character Table of the group $D_2(222)$*

$D_2(222)$	#	1	2_z	2_y	2_x	functions
A	Γ_1	1	1	1	1	x^2,y^2,z^2
B_1	Γ_3	1	1	-1	-1	z,xy,J_z
B_2	Γ_2	1	-1	1	-1	y,xz,J_y
B_3	Γ_4	1	-1	-1	1	x,yz,J_x

$\psi \sim (\Gamma_1, \Gamma_2, \Gamma_1, \Gamma_3)^T \sim (s, p_y, s, p_z)^T$

0.2 Find the matrix reps of all generators

No.	(x,y,z) form	Matrix form	Symmetry operation	
			ITA	Seitz
1	-x,-y,z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 0,0,z	2_{001}
2	-x,y,-z	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	2 0,y,0	2_{010}

$$g_1\,\psi = g_1 \begin{pmatrix} s \\ p_y \\ s \\ p_z \end{pmatrix} = \begin{pmatrix} s \\ -p_y \\ s \\ p_z \end{pmatrix} \Rightarrow g_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix};\ (C_{2\,z})$$

$$g_2\,\psi = g_2 \begin{pmatrix} s \\ p_y \\ s \\ p_z \end{pmatrix} = \begin{pmatrix} s \\ p_y \\ s \\ -p_z \end{pmatrix} \Rightarrow g_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix};\ (C_{2\,y})$$

g3 = K; (*TRS*)

1 Derive the k.p model

1.1 Initialize the k.p Hamiltonian

1.2 C_{2y} ($k_x \to -k_x$, $k_y \to k_y$, $k_z \to -k_z$)

```
H=H1+H2+H3;
dHC2y=(g2.H.Inverse[g2])-(H/.{kp→-km,km→-kp,kz→-kz});
MatrixForm[Collect[dHC2y,{kp,km,kz}]]
```

$$\left(\begin{array}{c} (es13 - es13s)\ km^2 + (-es13 + es13s)\ kp^2 \\ km\ (a121s + a122s + (b121s - b122s)\ kz) + kp\ (a121s + a122s + (-b121s + b1\ldots \\ (b132s - b133s)\ km^2 + (-b132s + b133s)\ kp^2 + 2\ a131s\ kz \\ -2\ a141s - 2\ b144s\ km\ kp - 2\ b141s\ kz^2 + kp^2\ (-b142s - b143s + (c141s - c142s)\ kz) + km^2\ (-b142s - \ldots \end{array}\right.$$

```
es13s = es13; epy3s = epy3; es23s = es23; epz3s = epz3;
a122 = -a121; a131 = 0; a141 = 0; a232 = -a231; a242 = a241; a341 = 0;
a122s = -a121s; a131s = 0; a232s = -a231s; a141s = 0; a242s = a241s; a341s = 0; epz3s = epz3;

b122 = b121; b133 = b132; b143 = -b142; b144 = 0; b141 = 0;
b232 = b231; b242 = -b241; b343 = -b342; b344 = 0; b341 = 0;
b122s = b121s; b133s = b132s; b143s = -b142s; b144s = 0; b141s = 0;
b232s = b231s; b242s = -b241s; b343s = -b342s; b344s = 0; b341s = 0;

c142 = c141; c142s = c141s;

MatrixForm[Simplify[dHC2y]]
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

1.3 TRS ($k_x \to -k_x$, $k_y \to -k_y$, $k_z \to -k_z$)

```
dHt=(Transpose[H]) - (H/.{kp → -kp, km → -km, kz → -kz});
MatrixForm[Collect[dHt,{kp,km,kz}]]
```

```
(                                                    0
                          km (a121 - a121s + (b121 - b121s) kz) + kp (-a121 + a121s + (b1
                   a130 - a130s + (b132 - b132s) km² + (b134 - b134s) km kp + (b132 - b132s)
 (a142 + a142s) kz + (c143 + c143s) km kp kz + (c144 + c144s) kz³ + km² (-b142 - b142s + (c141 + c1
```

```
a121s=a121;a130s=a130;a142s=-a142;a231s=a231;a241s=-a241;a342s=-a342;

b121s=b121;b134s=b134;b132s=b132;b131s=b131;b142s=-b142;b241s=-b241;b342s=-b342;b231s=b231;

c143s=-c143;c141s=-c141;c144s=-c144;

MatrixForm[Collect[dHt,{kp,km,kz}]]
```

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

```
kp=kx+ⅈ ky;
km=kx-ⅈ ky;
MatrixForm[Collect[H,{kx,ky,kz}]]
```

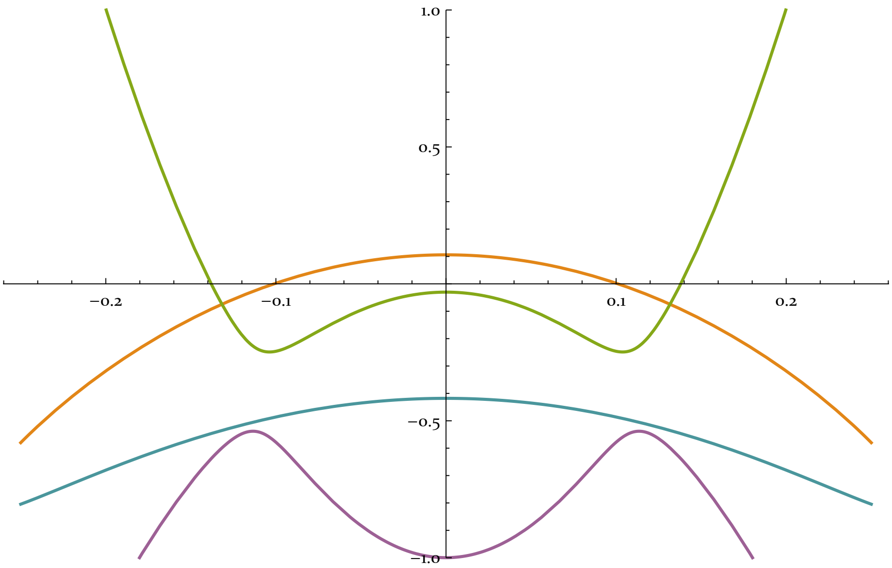
```
(           es10 + (es11 + 2 es13) kx² + (es11 - 2 es13) ky² + es12 kz²
                              2 ⅈ a121 ky + 2 b121 kx kz                                  epy0 + (epy1
           a130 + (2 b132 + b134) kx² + (-2 b132 + b134) ky² + b131 kz²
 4 ⅈ b142 kx ky - a142 kz + (-2 c141 - c143) kx² kz + (2 c141 - c143) ky² kz - c144 kz³
```

2 Plot bands along some high-symmetry paths

```
ClearAll["Global`*"]
H= ( e10+e11 kx^2+e12 ky^2+e13 kz^2                                              -2 i a121 ky+2
     2 i a121 ky+2 b121 kx kz                                                    e20+e21 kx^2+e22
     a130+b131 kx^2+b132 ky^2+b133 kz^2                                          2 i a231 ky+2
     4 i b142 kx ky-a142 kz+(-2 c141-c143) kx^2 kz+(2 c141-c143) ky^2 kz-c144 kz^3   -2 a241 kx+2 i

ky=0;kz=0;
{e10,e20,e30,e40}={-0.976,-0.418,-0.054,0.106};
{e11,e21,e31,e41}={49.26,-8.7,-28.7,-8.46};
{a130,b131,a241}={0.15,0,0.49};
MatrixForm[H]
Bd=Eigenvalues[H];
XGX=Plot[{Bd[[1]],Bd[[2]],Bd[[3]],Bd[[4]]},{kx,-0.25,0.25},PlotRange→{-1,1}];
Show[XGX]
```

$$\begin{pmatrix} -0.976+49.26\,kx^2 & 0 & 0.15 & 0 \\ 0 & -0.418-8.7\,kx^2 & 0 & 0.98\,kx \\ 0.15 & 0 & -0.054-28.7\,kx^2 & 0 \\ 0 & -0.98\,kx & 0 & 0.106-8.46\,kx^2 \end{pmatrix}$$



Assignments:

$O_h + t_{2g} / F_{3/2g}$ (Cu_2S)

(Be_2Se_3)

($Sm\ B_6$)

(Na_3Bi)

($HgCr_2Se_4$)

2, Magnetic Field Applied

3, Strain Applied