Lecture 11

Reminder: HW 2 due Thursday

$$G_k = \{ \{\bar{g}|\vec{d}\} \in G \mid \bar{g}k \equiv k \text{ modulo } \vec{Y} \}$$

set of elements that leave fixed the representation $\vec{k}$ of the Bravais lattice

① G_k is symmorphic → $\rho_k(\{\bar{g}|\vec{t}\}) = \rho_k(\{E|\vec{t}\})\rho_k(\{\bar{g}|0\})$

$$= e^{-i\vec{k}\cdot\vec{t}}\rho_k(\{\bar{g}|0\})$$

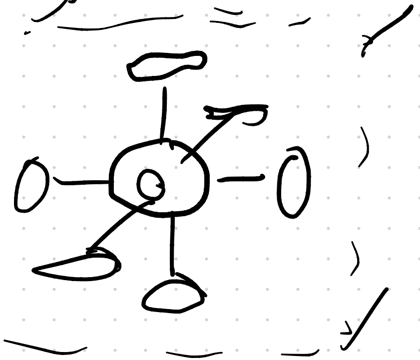
phase factor

representation of $\bar{G}_k = G_k/T$

② G_k is nonsymmorphic

Case 1 example P432

$\vec{k} = \vec{0}$ (Γ point) $\quad G_\Gamma = \cancel{P}432$, $\quad \bar{G}_\Gamma = 432$



Valence electrons

$\{ |d \text{ orbitals}\rangle \}$

$|l=2, m\rangle$

Character table

	1	4	2_1	3	2_{110}
A_1	1	1	1	1	1
A_2	1	-1	1	1	-1
E	2	0	2	-1	0
T_2	3	-1	-1	0	1
T_1	3	1	-1	0	-1

Absent other atoms, states transform in $\rho_{l=2}$ of $SO(3)$

$$\rho_{l=2}(\hat{n},\theta) = e^{-\hat{n}\cdot\vec{J}\theta}$$

$$J_z = \begin{pmatrix} 2 & & & & \\ & 1 & & & \\ & & 0 & & \\ & & & -1 & \\ & & & & 2 \end{pmatrix} \qquad J_x = \frac{1}{2}\begin{pmatrix} 0 & 2 & & & \\ 2 & 0 & \sqrt{6} & & \\ & \sqrt{6} & 0 & \sqrt{6} & \\ & & \sqrt{6} & 0 & 2 \\ & & & 2 & 0 \end{pmatrix}$$

$$J_y = \frac{1}{2i}\begin{pmatrix} 0 & 2 & & & \\ -2 & 0 & \sqrt{6} & & \\ & -\sqrt{6} & 0 & \sqrt{6} & \\ & & -\sqrt{6} & 0 & 2 \\ & & & -2 & 0 \end{pmatrix}$$

$$h_{mm'}(k=0) = \langle l=2\, m | H | l=2\, m' \rangle$$

$\rightarrow$ How does {Valence states} decompose into irreps of 432

$432 < SO(3) \leftarrow \rho_{l=2}$ is a representation of $SO(3)$

Given a representation of $SO(3)$ $\rho : SO(3) \to U(V)$

we can construct $\eta : 432 \to U(V)$ by <u>restriction</u>

$$\eta(g \in 432) = \rho_{\ell=2}(g) \quad \text{for } g \in 432$$

$$\eta = \rho_{\ell=2} \downarrow 432$$

5d reducible rep of 432

irreducible 5-d rep of $SO(3)$

We can use characters to find how η reduces

$$\chi_\eta(g) = \mathrm{tr}[\eta(g)] = \mathrm{tr}[\rho_{\ell=2}(g)]$$

$$\eta(E) = e^{-i0} = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \rightarrow \chi_\eta(E) = 5$$

$$\eta(C_{4z}) = e^{-i\frac{\pi}{2}J_z} = \begin{pmatrix} -1 & & & & \\ & -i & & & \\ & & 1 & & \\ & & & i & \\ & & & & -1 \end{pmatrix} \rightarrow \chi_\eta(C_{4z}) = -1$$

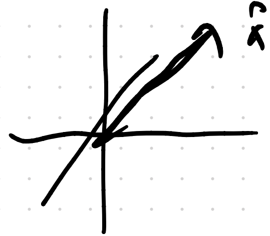
$$\eta(C_{2t}) = e^{-i\pi J_z} = \begin{pmatrix} 1 & & & & \\ & -1 & & & \\ & & 1 & & \\ & & & -1 & \\ & & & & 1 \end{pmatrix} \rightarrow \chi_\eta(C_{2t}) = +1$$

Trick for the remaining two

$$\chi_\eta(g) = tr[\rho_{l=2}(g)] \quad g \in 432$$

$$= \mathrm{tr}\left[\rho_{\ell=2}(g')\,\rho_{\ell=2}(g)\,\rho_{\ell=2}(g')\right]$$

$g \in 432$
$g' \in SO(3)$



Fun fact - all rotations by angle θ are conjugate in $SO(3)$

$$\Rightarrow \mathrm{tr}\left[\rho_{\ell=2}(C_{3,(111)})\right] = \mathrm{tr}\left[\rho_{\ell=2}(C_{3z})\right]$$

$$= \mathrm{tr}\left[\begin{pmatrix} e^{-4\pi i/3} & & & & \\ & e^{-2\pi i/3} & & & \\ & & 1 & & \\ & & & e^{2\pi i/3} & \\ & & & & e^{4\pi i/3} \end{pmatrix}\right] = 1 + 2\cos\frac{2\pi}{3} + 2\cos\frac{4\pi}{3} = -1$$

$$\chi_\eta(C_{2\,\hat{x}+\hat{y}}) = \chi_\eta(C_{2z}) = +1$$

$$\chi_\eta = \begin{array}{ccccc} 1 & 4 & 2_{100} & 3 & 2_{110} \\ \hline \end{array}$$
$$\chi_\eta = \begin{pmatrix} 5 & -1 & 1 & -1 & 1 \end{pmatrix}$$

	1	4	2_1	3	2_{110}
A_1	1	1	1	1	1
A_2	1	-1	1	1	-1
E	2	0	2	-1	0
T_2	3	-1	-1	0	1
T_1	3	1	-1	0	-1

inner product

$$\langle \chi_\eta, \chi_i \rangle = \frac{1}{24} \sum_{g \in G} \chi_\eta^*(g) \chi_i(g)$$

$$= \frac{1}{24} \Big[\chi_\eta^*(E)\chi_i(E) + 6\chi_\eta^*(C_{4z})\chi_i(C_{4z}) + 3\chi_\eta^*(C_{2z})\chi_i(C_{2z})$$
$$+ 8\chi_\eta^*(C_{3z})\chi_i(C_{3z}) + 6\chi_\eta^*(C_{2110})\chi_i(C_{2110}) \Big]$$

$$\langle \chi_\eta, \chi_{A_1} \rangle = \frac{1}{24}\left(5 + (-6) + 3 - 8 + 6\right) = 0$$

$$\langle \chi_\eta, \chi_{A_2} \rangle = 0$$

$$\langle \chi_\eta, \chi_E \rangle = \frac{1}{24}(10 + 6 + 8) = 1$$

$$\langle \chi_\eta, \chi_{T_2} \rangle = \frac{1}{24}(15 + 6 - 3 + 6) = 1$$

$$\chi_\eta = \chi_E + \chi_{T_2}$$

$$\eta = \rho_{\ell=2} \downarrow 432 \cong E \oplus T_2$$

$$\{|\ell=2, m\rangle\} \xrightarrow{\text{basis trans}} \{|1_E\rangle, |2_E\rangle, |1_{T_2}\rangle, |2_{T_2}\rangle,$$

$|3_{T_2}\rangle \}$

in this basis

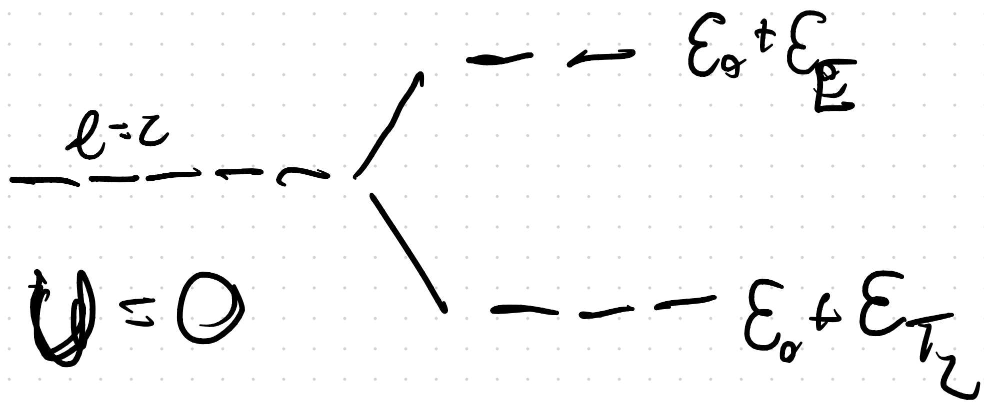
$$\eta(g) = \begin{array}{c} \begin{array}{ccccc} 1_E & 2_E & 1_{T_2} & 2_{T_2} & 3_{T_2} \end{array} \\ \left(\begin{array}{c|c} \rho_E(g) & 0 \\ \hline 0 & \rho_{T_2}(g) \end{array} \right) \end{array} \begin{array}{c} 1_E \\ 2_E \\ 1_{T_2} \\ 2_{T_2} \\ 3_{T_2} \end{array}$$

$$\langle a_E | H | b_E \rangle = (\varepsilon_0 + \varepsilon_E)\delta_{ab}$$

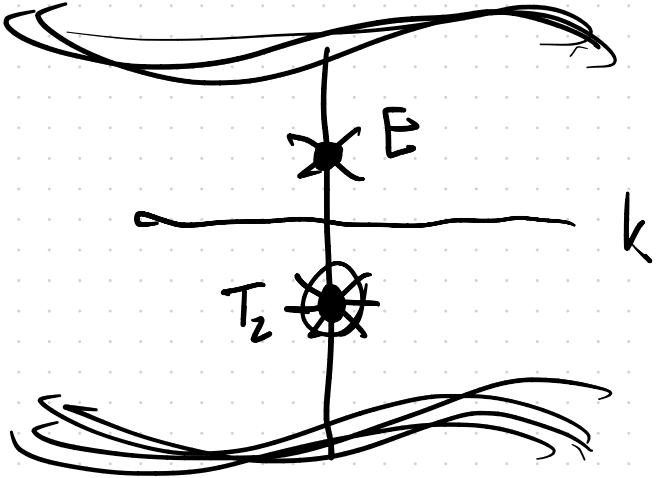
$$\langle a_{T_2} | H | b_{T_2} \rangle = (\varepsilon_0 + \varepsilon_{T_2})\delta_{ab}$$

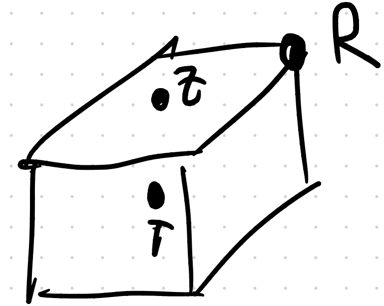
$$h(k=0) = \begin{array}{c} \\ \\ \\ \\ \\ \end{array}\begin{array}{cc|ccc} 1_E & 2_E & 1_{T_2} & 2_{T_2} & 3_{T_2} \end{array}$$

$$h(k=0) = \left(\begin{array}{cc|ccc} \varepsilon_0+\varepsilon_E & 0 & & & \\ 0 & \varepsilon_0+\varepsilon_E & & 0 & \\ \hline & & \varepsilon_0+\varepsilon_{T_2} & 0 & 0 \\ & 0 & 0 & \varepsilon_0+\varepsilon_{T_2} & 0 \\ & & 0 & 0 & \varepsilon_0+\varepsilon_{T_2} \end{array}\right) \begin{array}{c} 1_E \\ 2_E \\ 1_{T_2} \\ 2_{T_2} \\ 3_{T_2} \end{array}$$



"Crystal field splitting"



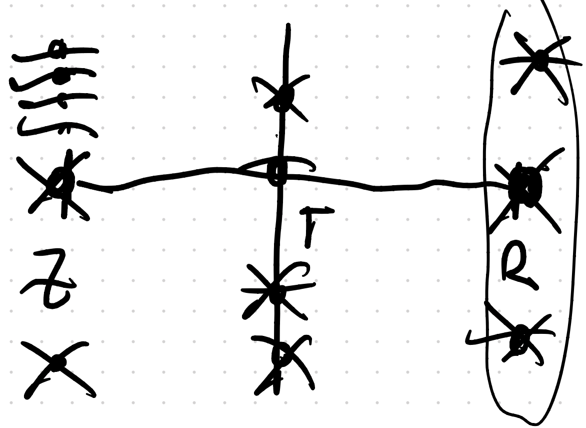


$G_Z = P422$

$\bar{G}_Z = 422$

ρ	dimension
A_1	1
A_2	1
B_1	1
B_2	1
E	2

can have 1 fold or twofold degenerate states



Group theory can fix the degeneracies of states, but not their energies

(2) G_k nonsymmorphic

$$G_k = \bigcup_{i=0}^{n-1} T\{\bar{g}_i | \vec{d}_i\} \qquad \{\bar{g}_i, i=0,\dots,n-1\} = \overline{G_k}$$

at least one of $\vec{d}_i$ is a fraction of a Bravais lattice translation

→ there is some $g_a = \{\bar{g}_a | \vec{d}_a\}$, $\{\bar{g}_b | \vec{d}_b\} = g_b$

$$g_a g_b = \{\bar{g}_a \bar{g}_b | \vec{d}_a + \bar{g}_a \vec{d}_b\} = \{E | \vec{t}_{ab}\}\{\overline{g_a g_b} | \vec{d}_{ab}\}$$

products of coset representative = (nonzero translation) × another coset representative

Ex: $g_a = g_b = \{C_{2z} | \frac{1}{2}\hat{z}\}$

$$g_a g_b = \{E | \hat{z}\}\{E | \vec{0}\}$$

↳ in any little group representation $e^{-ik\cdot\vec{t}_{ab}}$

$$\rho_k(g_a)\rho_k(g_b) = \rho_k(\{E|t_{ab}\})\rho_k(\{\bar{g}_a\bar{g}_b|\vec{\tau}_{ab}\})$$

but in $\bar{G}_k$ $\quad \eta(\bar{g}_a)\eta(\bar{g}_b) = \eta(\bar{g}_a\bar{g}_b)$

To accomodate this: still work $\bar{G}_k$ but generalize our idea of representations

$$\rho_k : \bar{G}_k \to U(V)$$

$$\rho_k(\bar g_1)\rho_k(\bar g_2) = e^{ic(\bar g_1,\bar g_2)}\rho_k(\bar g_1\bar g_2)$$

generalises the homomorphism rule

$$\Big(\rho_k(\bar g_1)\big(\rho_k(\bar g_2)\big)\rho_k(\bar g_3)\Big) \longrightarrow \rho_k(\bar g_1)\, e^{ic(\bar g_2,\bar g_3)}\rho_k(\bar g_2\bar g_3)$$

$$e^{ic(\bar g_1,\bar g_2)}\rho_k(\bar g_1\bar g_2)\rho_k(\bar g_3)$$

$$= e^{ic(\bar g_1,\bar g_2)+ic(\bar g_1\bar g_2,\bar g_3)}\rho_k(\overline{g_1g_2g_3})$$

$$= e^{ic(\bar g_2,\bar g_3)+ic(\bar g_1,\overline{g_2g_3})}\rho_k(\overline{g_1g_2g_3})$$

$$c(\bar g_1,\bar g_2)+c(\bar g_1\bar g_2,\bar g_3)-c(\bar g_2,\bar g_3)-c(\bar g_1,\bar g_2\bar g_3) = 0 \mod 2\pi$$

"cocycle condition"

a map $\rho_k : \bar{G}_k \to U(V)$ s.t. $\rho_k(\bar{g}_1)\rho_k(\bar{g}_2) = e^{ic(\bar{g}_1,\bar{g}_2)}\rho_k(\bar{g}_1\bar{g}_2)$

w/ c satisfying the cocycle condition

is a called a <u>projective representation</u>

For a nonsymmorphic little group

- Fix a set of coset representatives $\{\bar{g}_i | \vec{d}_i\}$

$$\{\bar{g}_i | \vec{d}_i\}\{\bar{g}_j | \vec{d}_j\} = \{\bar{g}_i\bar{g}_j | \vec{d}_i + \bar{g}_i\vec{d}_j\}$$

$$= \{E \mid t_{ij}\}\{\bar{g}_i \bar{g}_j \mid \vec{d}_{ij}\}$$

$$\vec{t}_{ij} = \bar{g}_i \vec{d}_j + \vec{d}_i - \vec{d}_{ij}$$

$$C(\bar{g}_i, \bar{g}_j) = -k \cdot t_{ij}$$