Lecture 26

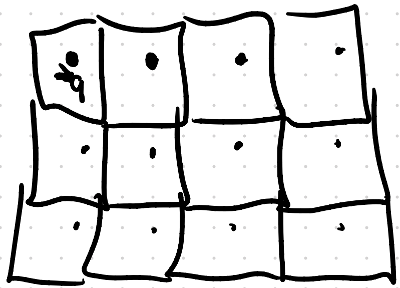
Final presentation scheduling

11/28 - 4

11/30 - 4

12/5 - 3

Will randomly assign an order and email everyone tonight!



$|W_{n0}\rangle$ – atomic-like orbitals centered at $\vec{r} = \vec{0} + \vec{q}$

$|W_{n\vec{R}}\rangle = U_{\vec{R}} |W_{n0}\rangle$ Bravais lattice T

space group G

$G \supset G_q$ – site symmetry group of $\vec{q}$

$G_q = \{ g \in G \mid g\vec{q} = \vec{q} \}$

$|W_{n0}\rangle$ transform in a representation ρ of G_q

$g_q \in G_q \qquad U_{g_{\vec{q}}} |W_{n\sigma}\rangle = \sum_m |W_{m\sigma}\rangle \rho_{mn}(g_{\vec{q}})$

$G \supset TG_q \qquad \{E|t\} g_{\vec{q}} \in TG_q \qquad g_q = \{\bar{g}|\vec{d}\}$

$$U_{\{E|t\} g_{\vec{q}}} |W_{n\vec{R}}\rangle = |W_{m\,\bar{g}\vec{R}+t}\rangle \rho_{mn}(g_q)$$

What about other elements of the space group

Look at the coset decomposition of G w.r.t TG_q

$$G = TG_q \cup g_2 TG_q \cup g_3 TG_q \cup \cdots \cup g_N TG_q$$

$g_1 = \{E|\vec{0}\}$

$$[G : TG_q] = [\bar{G} : G_q] \qquad \frac{|\bar{G}|}{|G_q|} = N \text{ finite}$$

$g_2, g_3, \ldots g_N \notin TG_q$

$$g = \{\bar{g}|\vec{d}\}$$

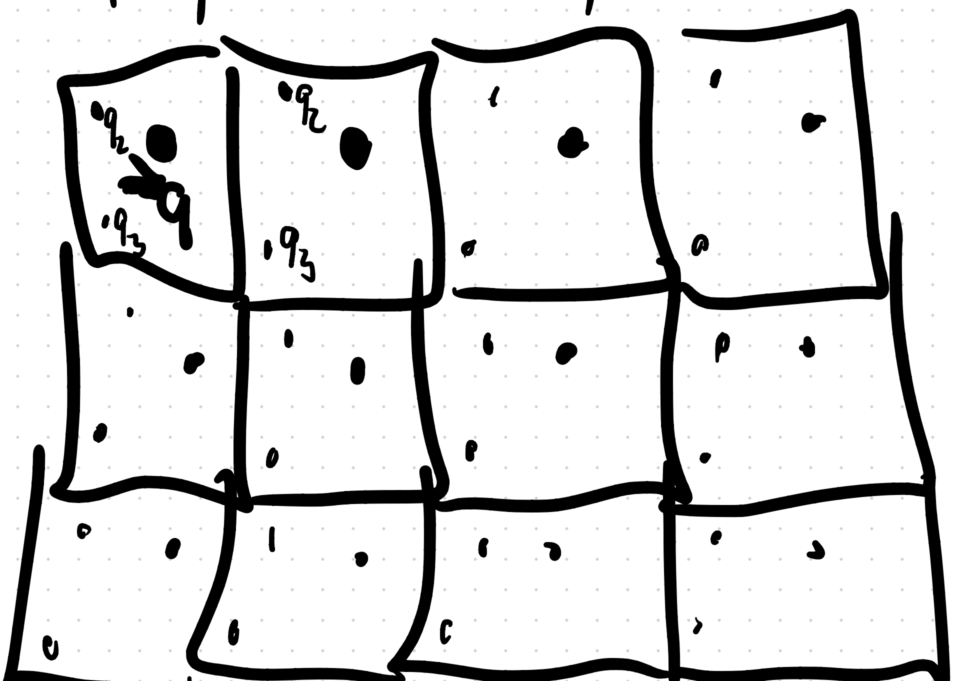
$$g_i \vec{q} = \vec{q}_i \qquad \vec{q}_1 = \vec{q}$$

$$(g\vec{q})_i = O(\bar{g})_{ij} q_j + d_i$$

$\vec{q}_{i\neq 1} \neq \vec{q} + \vec{R}$ for any Bravais lattice vector

("usual" rotation matrix

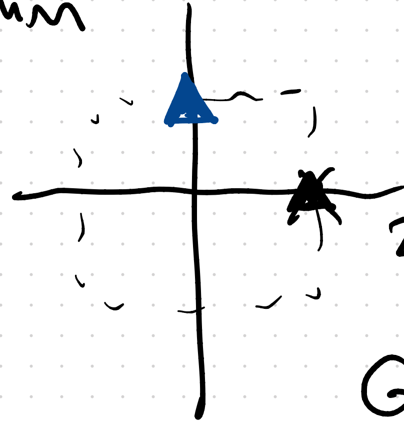
g_i map $\vec{q}$ to other points in the unit cell)



→ We have atoms and orbitals

$$U_{g_i}|W_{n\vec{0}}\rangle \equiv |W_{n\vec{0}i}\rangle$$

Ex $p4mm$



$2c \quad \left(\frac{a}{2}, 0\right)$

$$G_{2c} = \langle M_x, \{C_{2z} | a\hat{x}\} \rangle$$

Coset decomposition

$$p4mm = T G_{2c} \cup C_{4z} T G_{2c}$$

$g_1 = \{E|\vec{0}\}$

$g_2 = \{C_{4z}|0\}$

⇒ We can build a representation of G in position space

Basis functions $|W_{n\vec{R}i}\rangle = U_{\vec{R}} U_{g_i} |W_{n\vec{0}}\rangle$

Consider $g = \{\bar{g}|\vec{d}\} \in G$

$U_g |W_{n\vec{R}i}\rangle$

$gg_i = g_j t_{ij} h_{ij}$

coset representative

bravais lattice translation

$\in G_q$

From coset decomposition

$$g = g_j t'_{ij} h_{ij} g_i^{-1} = t_{ij} g_j h_{ij} g_i^{-1}$$

$$t_{ij} = g_j t'_{ij} g_j^{-1}$$

Note: $g(g_i \vec{q}) = t_{ij} g_j \underline{h_{ij}} \cancel{g_i^{-1}} (\cancel{g_i} \underline{\vec{q}})$

$$t_{ij}[\vec{v}] = \vec{v} + \vec{t}_{ij}$$

$$= t_{ij} g_j \vec{q}$$

$$\boxed{\vec{t}_{ij} = g(g_i \vec{q}) - g_j \vec{q}} \quad g = t_{ij} g_j h_{ij} g_i^{-1}$$

$$U_g |W_{n\vec{R}i}\rangle = U_g U_{\vec{R}} U_{g_i} |W_{n0}\rangle$$

$$= U_{\bar{g}\vec{R}} U_g U_{g_i} |W_{n0}\rangle$$

$$= U_{\bar{g}\vec{R}} U_{gg_i} |W_{n0}\rangle$$

$$= U_{\bar{g}\vec{R}} U_{t_{ij}} U_{g_j} U_{h_{ij}} |W_{n0}\rangle$$

$$= \sum_m U_{\bar{g}\vec{R}} U_{t_{ij}} U_{g_j} |W_{m0}\rangle \rho_{mn}(h_{ij})$$

$$U_g |W_{nRi}\rangle = \sum_m |W_{m\,\bar{g}\vec{R}+t_{ij}\,j}\rangle \rho_{mn}(h_{ij})$$

This gives a representation of G using

① $G = \bigcup_{i=1}^{N} g_i T G_q$

② a representation ρ of G_q

$\rho \uparrow G$ - representation of G <u>induced</u> from ρ

"band representation"

Bloch functions $|\psi_{ni\vec{k}}\rangle = \sum_{R} e^{i\vec{k}\cdot\vec{R}} |W_{n\vec{R}i}\rangle$

$$\underline{U_g|\psi_{ni\vec{k}}\rangle} = \sum_m |\psi_{mj\bar{g}k}\rangle \rho_{mn}(h_{ij}) e^{-i\bar{g}k\cdot t_{ij}}$$

Sewing matrix

$$\langle\psi_{mj\bar{g}k}|U_g|\psi_{nik}\rangle = B_k^{(mj),(ni)}(g) = e^{-i\bar{g}k\cdot t_{ij}} \rho_{mn}(h_{ij})$$

The band representation determines the little group representations @ high symmetry points

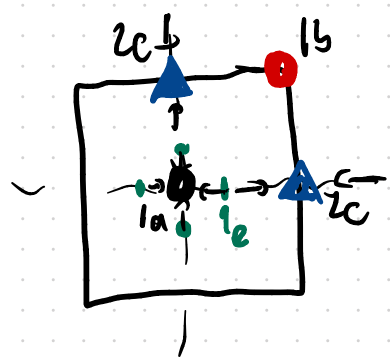
How many band representations are there & how do we organize them

① if $\rho = \rho_1 \oplus \rho_2$ is reducible

$$\rho \uparrow G = \rho_1 \uparrow G \oplus \rho_2 \uparrow G$$

we need to only consider irreps of $G_{\vec{q}}$

Ex: p4mm



- We only need to consider one $\vec{q}$ in every orbit [i.e. $(\frac{a}{2},0)$ and not $(0,\frac{a}{2})$]

$q_e = (\underline{u}\,0\,0)$ $\quad u \in (\underline{0}, \tfrac{1}{2})$ 4e position

$\boxed{G_{q_e}} = \langle M_x \rangle$

$G_{q_e} \subset G_{1a}$

$G_{q_e} \subset G_{2c}$

- Maximal Wyckoff positions - points with higher symmetry than their neighbors

All band reps are induced from sums of irreps of site symmetry groups at Maximal Wyckoff positions

↳ Elementary band representations

$\underline{|1\rangle}$ $\underline{|2\rangle}$ $\underline{|3\rangle}$ $\underline{|4\rangle}$

$$|a\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right)$$

$$|b\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right)$$

$$|c\rangle = \frac{1}{\sqrt{2}}\left(|3\rangle + |4\rangle\right)$$

$$|d\rangle = \frac{1}{\sqrt{2}}\left(|3\rangle - |4\rangle\right)$$