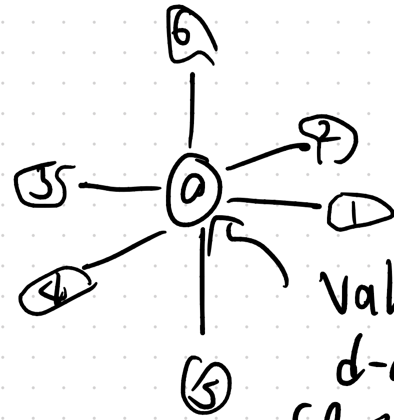
Lecture 10

Recap



Valence d-orbital ($l=2$ states)

$$H = H_0 + V(\vec{x})$$

Hamiltonian for the isolated central atom

the ionic potential from nuclei 1-6

Symmetry group: 432

$\overline{G}$ $\qquad g \in \overline{G}, \; V(g^{-1}x) = V(x)$

$$\langle lm | H_0 | lm' \rangle = \varepsilon_0 \delta_{mm'} = \begin{pmatrix} \varepsilon_0 & & & & \\ & \varepsilon_0 & & & \\ & & \varepsilon_0 & & \\ & & & \varepsilon_0 & \\ & & & & \varepsilon_0 \end{pmatrix}$$

$l=2$

Find the corrections to the energy to first order in V

degenerate perturbative theory

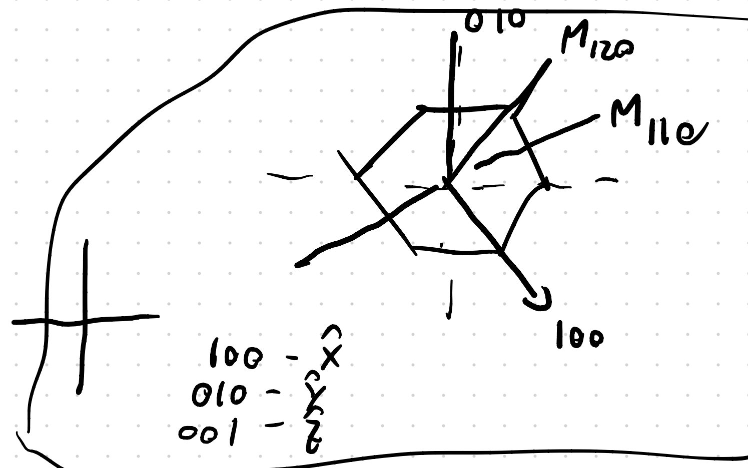
diagonalise $\boxed{\langle lm | V | lm' \rangle}$

$\{ |l=2, m\rangle \}$ transform in the $\rho_{l=2}$ rep of $SO(3)$

$\eta = \rho_{l=2} \downarrow \bar{G}$

$\underline{\eta(g \in \bar{G})} = \rho_{l=2}(g)$

$\chi_\eta(g) = \mathrm{tr}\, \rho_\eta(g)$



100 - $\hat{x}$
010 - $\hat{y}$
001 - $\hat{z}$

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

$$\rightarrow \boxed{\eta \cong \rho_E \oplus \rho_{T_2}}$$

$$\{|l=2\,m\rangle\} \longrightarrow \{|1_E\rangle, |2_E\rangle, |1_{T_2}\rangle, |2_{T_2}, 3_{T_2}\rangle\}$$

$$\boxed{[V]} = \begin{array}{cc} & \begin{array}{ccccc} 1_E & 2_E & 1_{T_2} & 2_{T_2} & 3_{T_2} \end{array} \\ & \left(\begin{array}{c|c} V_{EE} & \boxed{V_{ET_2} = 0} \\ \hline V_{T_2E} = 0 & V_{T_2T_2} \end{array}\right) \end{array} \begin{array}{c} 1_E \\ 2_E \\ 1_{T_2} \\ 2_{T_2} \\ 3_{T_2} \end{array}$$

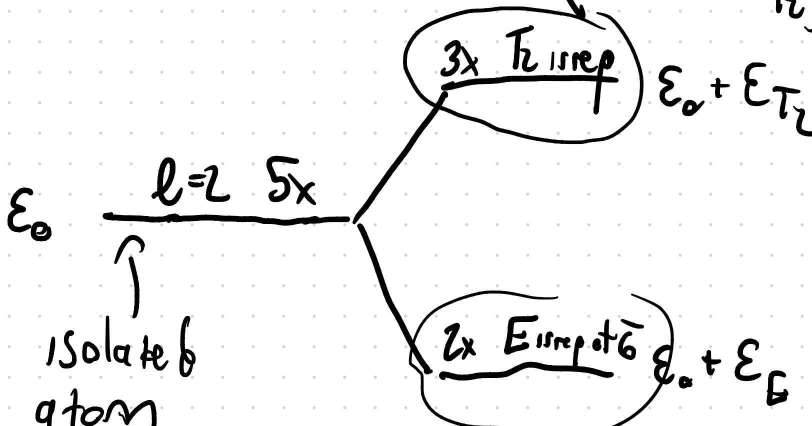
V_{ET_2} : T_2 rep $\to$ E rep

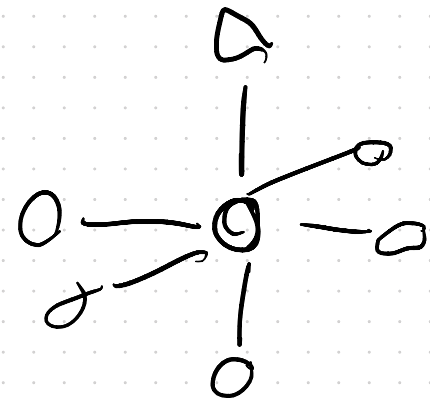
$\downarrow$ Schur's Lemma

$$0 = V_{T_2E}$$

$$V_{EE} = \begin{pmatrix} \varepsilon_E & \\ & \varepsilon_E \end{pmatrix} \qquad \varepsilon_E \neq \varepsilon_{T_2} \quad \text{generally}$$

$$V_{T_2T_2} = \begin{pmatrix} \varepsilon_{T_2} & & \\ & \varepsilon_{T_2} & \\ & & \varepsilon_{T_2} \end{pmatrix}$$





"Crystal field splitting"

$$\underline{[V, \eta(g)] = 0}$$

$$\eta(g) = \left(\begin{array}{c|c} \rho_E(g) & 0 \\ \hline 0 & \rho_{T_2}(g) \end{array}\right)$$

$$V = \left(\begin{array}{c|c} V_{EE} & V_{ET_2} \\ \hline V_{T_2E} & V_{T_2T_2} \end{array}\right)$$

$$V\eta(g) = \begin{pmatrix} V_{EE}\,\rho_E(g) & V_{ET_2}\,\rho_{T_2}(g) \\ V_{T_2E}\,\rho_E(g) & V_{T_2T_2}\,\rho_{T_2}(g) \end{pmatrix}$$

$$\eta(g)V = \left(\begin{array}{c|c} \rho_E(g)V_{EE} & \rho_E(g)V_{ET_2} \\ \hline \rho_{T_2}(g)V_{T_2E} & \rho_{T_2}V_{T_2E} \end{array}\right) \Rightarrow \begin{array}{l} [V_{EE}, \rho_E(g)] \\ [V_{T_2T_2}, \rho_{T_2}(g)] \\ \\ V_{ET_2}\rho_{T_2}(g) = \rho_E(g)V_{ET_2} \\ V_{T_2E}\,\rho_E(g) = \rho_{T_2}(g)V_{T_2E} \end{array}$$

"International Tables for Crystallography Vol A"

Bradley & Cracknell

Now: lets add translations and use space groups to study band structure

crystal w/ space group symmetry G Bravais lattice $T \triangleleft G$

pt group $\bar{G} = G/T$

Translation symmetry: Bloch's theorem $H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$

$$u_t|\psi_{nk}\rangle = e^{-i\vec{p}\cdot\vec{t}/\hbar}|\psi_{nk}\rangle$$
$$= e^{-ik\cdot\vec{t}}|\psi_{nk}\rangle$$

in other words: $\mathcal{H} = \bigcup_{k \in BZ} |\varphi_{a\vec{k}}\rangle$

$$U_t |\varphi_{ak}\rangle = e^{-ik\cdot\vec{t}} |\varphi_{ak}\rangle$$

$$\langle \varphi_{bk'} | H | \varphi_{ak} \rangle \propto \delta_{kk'}$$

What about other symmetries $\{\bar{g} | \vec{d}\} \in G$

$$\bar{g} \in \bar{G}$$

let $U_{\{\bar{g}|d\}}$ be a unitary operator on $\mathcal{H}$ that implements this symmetry

$$\{\bar{g}|\vec{d}\} \in G \Rightarrow [H, U_{\{\bar{g}|\vec{d}\}}] = 0$$

$\boxed{U_{\{\bar{g}|\vec{d}\}} |\varphi_{a\vec{k}}\rangle}$ $\Leftarrow$ what state is this?

in particular, what is the $\vec{k}$ for this state

$$U_{\{E|\vec{t}\}} \left(U_{\{\bar{g}|\vec{d}\}} |\varphi_{ak}\rangle \right) = U_{\{E|\vec{t}\}\{\bar{g}|\vec{d}\}} |\varphi_{ak}\rangle$$

but $\{E|\vec{t}\}\{\bar{g}|\vec{d}\} = \{\bar{g}|\vec{d}+\vec{t}\}$

$$= \underline{\{\bar{g}|\vec{d}\}\{E|\bar{g}^{-1}\vec{t}\}}$$

$$U_{\{\bar{g}|\vec{d}\}} U_{\{E|\bar{g}\vec{t}\}} |\varphi_{ak}\rangle = \underbrace{e^{-i\vec{k}\cdot(\bar{g}^{-1}t)}} \left(U_{\{\bar{g}|\vec{d}\}} |\varphi_{ak}\rangle \right)$$

$$\vec{k}\cdot(\bar{g}^{-1}\vec{t}) = (\bar{g}k)\cdot(\bar{g}\bar{g}^{-1}t) = \bar{g}k\cdot\vec{t}$$

$$U_{\{E|\vec{t}\}}\left(U_{\{\bar{g}|\vec{d}\}} |\varphi_{ak}\rangle \right) = e^{-i\bar{g}k\cdot\vec{t}} \left(U_{\{\bar{g}|\vec{d}\}} |\varphi_{ak}\rangle \right)$$

$$\boxed{U_{\{\bar{g}|\vec{d}\}} |\varphi_{ak}\rangle \text{ has crystal momentum } \bar{g}\vec{k}}$$

$$\bar{g}\vec{k} = R_{3\times3}(g)\cdot k$$

$\hookrightarrow$ 3×3 vector representation inherited from $O(3)$

$$U_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle = \sum_{bk'} |\varphi_{bk'}\rangle\langle\varphi_{bk'}|U_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle$$

$$= \sum_{b} |\varphi_{b\bar{g}k}\rangle\langle\varphi_{b\bar{g}k}|U_{\{\bar{g}|\vec{d}\}}|\varphi_{a\vec{k}}\rangle$$

(n, m, l - label eigenstates of H
a, b, c - label general states in Hilbert space)

$$= \sum_{b} |\varphi_{b\bar{g}k}\rangle \underbrace{B^{\vec{k}}_{ba}(\{\bar{g}|\vec{d}\})}_{\text{Sewing matrix for } \{\bar{g}|\vec{d}\}}$$

in the basis of eigenstates of H

$$U_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle = \sum_{m} |\psi_{m\bar{g}k}\rangle B^{\vec{k}}_{mn}(\{\bar{g}|\vec{d}\})$$

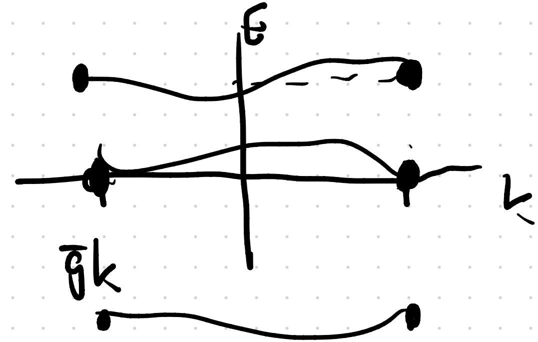
$$H\, u_{\{\bar{g}|\vec{d}\}} |\psi_{nk}\rangle = u_{\{\bar{g}|\vec{d}\}} H |\psi_{nk}\rangle$$

$$= E_{nk}\, u_{\{\bar{g}|\vec{d}\}} |\psi_{nk}\rangle$$

$$= \sum_m H |\psi_{m\bar{g}k}\rangle B^{\vec{k}}_{mn}(\{\bar{g}|\vec{d}\})$$

$$= \sum_m E_{m\bar{g}k} |\psi_{m\bar{g}k}\rangle \underline{B^{\vec{k}}_{mn}(\{\bar{g}|\vec{d}\})}$$

$$B^{\vec{k}}_{mn}(\{\bar{g}|\vec{d}\}) = 0 \quad \text{unless } E_{m\bar{g}k} = E_{n\vec{k}}$$



Something special happens when $\bar{g}k = \vec{k} + \vec{b}$

$\vec{b} \in$ reciprocal lattice

$$\bar{g}k = k + \vec{b} \quad (\bar{g}\vec{k} \equiv k \bmod \check{T})$$

$$e^{-i\bar{g}k\cdot t} = e^{-i(k+b)\cdot\vec{t}} = e^{-i\vec{k}\cdot\vec{t}}$$

$\Rightarrow \{|\varphi_{a\bar{g}k}\rangle\}$ and $\{|\varphi_{bk}\rangle\}$ span the same Hilbert space

$\rightarrow$ $B^{k}_{nm}(\{\bar{g}|\vec{d}\})$ is a map from a vector space to itself

Given some fixed $\vec{k}$ we define $G_k < G$

$$\boxed{G_k} = \left\{ \{\bar{g}|\vec{d}\} \in G \;\middle|\; \bar{g}\vec{k} \equiv \vec{k} \mod \check{T} \right\}$$

little group of $\vec{k}$

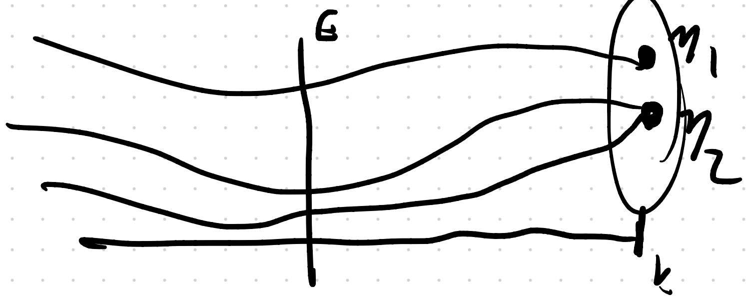
$$\left\{ B^{\vec{k}}_{nm}(\{\bar{g}|\vec{d}\}) \;\middle|\; \{\bar{g}|\vec{d}\} \in G_k \right\}$$ form a representation of G_k

Bloch's theorem + Schur's Lemma: for fixed $\vec{k}$
the eigenstates $\{|\psi_{nk}\rangle\}$ must decompose into irreps of G_k

$$\{ \{|\psi_{1nk}\rangle\}, \{|\psi_{2nk}\rangle\}, \dots \}$$
$$\uparrow \qquad\qquad \uparrow$$
$$\eta_1^k \qquad\qquad \eta_2^k$$

$$B^k = \begin{pmatrix} \eta_1 & & & \\ & \eta_2 & & \\ & & \ddots & \\ & & & \ddots \end{pmatrix}$$

$$H|\psi_{ink}\rangle = E_{ik}|\psi_{ink}\rangle$$



$\dim \eta_2 = 2$

- Little group representations protect degeneracies in the spectrum

$$\langle \psi_{nk} | H | \psi_{mk} \rangle B^k_{ml}(\{\bar{g}|\vec{d}\})$$

$$= \langle \psi_{nk} | H\, U_{\{\bar{g}|\vec{d}\}} | \psi_{lk} \rangle$$

$$= \langle \psi_{nk} | U_{\{\bar{g}|\vec{d}\}} H | \psi_{lk} \rangle$$

$$= B^{k}_{nm}(\{g\}|\{d\})\langle \psi_{mk}|H|\psi_{\ell k}\rangle$$