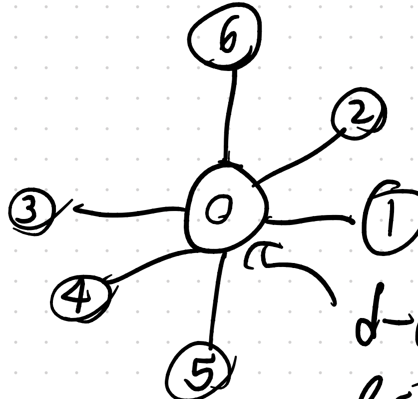
Lecture 10



d-orbital
$l=2$

$$H = H_0 + V(x)$$

H_0: Hamiltonian for the isolated atom

$V(x)$: ionic potential from nuclei 1-6

$\overline{G}$ Symmetry group 432 (octahedral group)

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

$$\langle 2,m | H_0 | 2m' \rangle = \begin{pmatrix} \varepsilon_0 & & & & 0 \\ & \varepsilon_0 & & & \\ & & \varepsilon_0 & & \\ & & & \varepsilon_0 & \\ 0 & & & & \varepsilon_0 \end{pmatrix}$$

Representations η of $\bar{G}$ $\eta = \rho_{\ell=2} \downarrow \bar{G}$

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

$\Rightarrow \eta \cong \rho_E \oplus \rho_{T_2}$

$\{|\ell=2, m\rangle\} \rightarrow \{|1_E\rangle, |2_E\rangle, |1_{T_2}\rangle + |2_{T_2}\rangle, |3_{T_2}\rangle\}$

in this basis

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

What about the matrix elements of V in this basis

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

$$[V]\eta(s) = \eta(s)[V]$$

$$\left(\begin{array}{c|c} V_{EE} & V_{ET_2} \\ \hline V_{T_2E} & V_{T_2T_2} \end{array}\right)\left(\begin{array}{c|c} \rho_E(s) & \\ \hline & \rho_{T_2}(s) \end{array}\right) = \left(\begin{array}{c|c} \rho_E(s) & \\ \hline & \rho_{T_2}(s) \end{array}\right)\left(\begin{array}{c|c} V_{EE} & V_{ET_2} \\ \hline V_{T_2E} & V_{T_2T_2} \end{array}\right)$$

$$V_{EE}\,\rho_E(s) = \rho_E(s)\,V_{EE} \xrightarrow{\text{Schur's lemma pt 2}} V_{EE} = \varepsilon_E \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

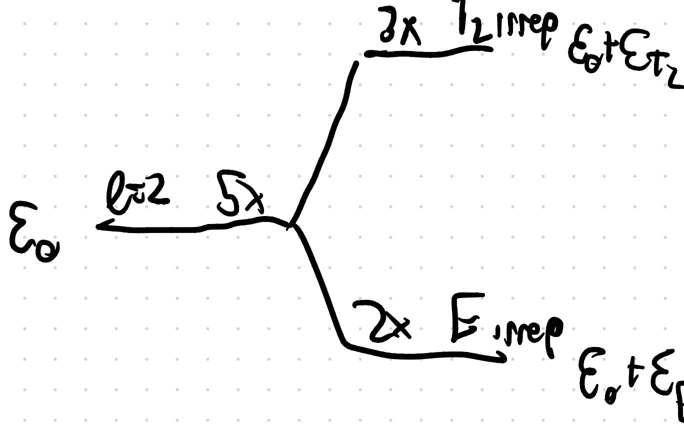
$$V_{T_2T_2}\,\rho_{T_2}(s) = \rho_{T_2}(s)\,V_{T_2T_2} \longrightarrow V_{T_2T_2} = \varepsilon_{T_2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$V_{ET_2}\,\rho_{T_2}(s) = \rho_E(s)\,V_{ET_2} \longrightarrow V_{ET_2} = 0$$

$V_{T_2 E} = 0$

$$[H] = [H_0] + [V] = \left(\begin{array}{cc|ccc} \varepsilon_0 + \varepsilon_E & & & & \\ & \varepsilon_0 + \varepsilon_E & & 0 & \\ \hline & & \varepsilon_0 + \varepsilon_{T_2} & & \\ & 0 & & \varepsilon_0 + \varepsilon_{T_2} & \\ & & & & \varepsilon_0 + \varepsilon_{T_2} \end{array}\right)$$

$\xrightarrow{V}$



← "crystal field splitting"

Lets add translation symmetry → space

group symmetry & band structure

Noninteracting H invariant under space group G

Bravais lattice $T \triangleleft G$

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

Translation symmetry alone $\rightarrow$ Bloch's theorem

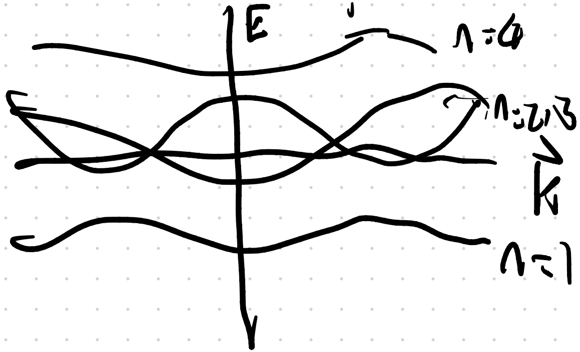
$$H|\psi_{n\vec{k}}\rangle = E_{nk}|\psi_{nk}\rangle$$

$$U_t|\psi_{nk}\rangle = e^{-ik\cdot\vec{t}}|\psi_{nk}\rangle$$

Hilbert space $\mathcal{H} = \bigcup_{\vec{k}\in BZ}\{|\varphi_{ak}\rangle\}$

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

$$\langle\varphi_{ak}|H|\varphi_{bk'}\rangle = h_{ab}(k)\delta_{kk'}$$



by Schur's lemma

What do symmetries like $\{\bar{g}|\vec{d}\} \in G$

$\Uparrow$

$\bar{G}$

do to Bloch states?

unitary operator $U_{\{\bar{g}|\vec{d}\}}$ on Hilbert space that implements this transformation

$$U_{\{\bar{g}|\vec{d}\}}\, \hat{X}\, U^{-1}_{\{\bar{g}|\vec{d}\}} = \bar{g}\hat{X} + \vec{d}$$

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

$U_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle \leftarrow$ What state is this?

in particular - How does this state transform under Bravais lattice translations

$\bar{g}k$?

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

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

$$= U_{\{\bar{g}|\vec{\alpha}\}} U_{\{E|\bar{g}^{-1}t\}} |\varphi_{ak}\rangle$$

$$= U_{\{\bar{g}|\vec{\alpha}\}} e^{-i\vec{k}\cdot\bar{g}^{-1}\vec{t}} |\varphi_{ak}\rangle$$

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

But $\cdot$ is invariant under all rotations and reflections

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

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

$U_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle$ transforms with $\bar{g}k$ irrep of T (has crystal momentum $\bar{g}k$)

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

a, b, c, ... label general basis states in Hilbert space

$$= \sum_{b} |\varphi_{b\bar{g}k}\rangle \underbrace{\langle\varphi_{b\bar{g}k}|U_{\{\bar{g}|\vec{d}\}}|\varphi_{ak}\rangle}_{B^{\vec{k}}_{ba}(\{\bar{g}|\vec{d}\})}$$

Sewing matrix for $\{\bar{g}|\vec{d}\}$

n, m, l, ... label energy eigenstates / bands

Can do the same thing in the basis $|\psi_{nk}\rangle$ of eigenstates of H

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

Sewing matrix in the band basis

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

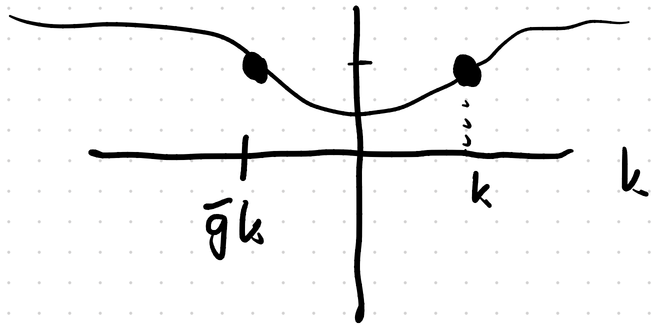
$$E_{nk} U_{\{g|\vec{d}\}}|\psi_{nk}\rangle = H\, U_{\{g|\vec{d}\}}|\psi_{nk}\rangle = H \sum_m |\psi_{m\bar{g}k}\rangle B_{mn}^{\vec{k}}(\{g|\vec{d}\})$$

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

$\Rightarrow$ $B_{mn}^{k}(\{\bar{g}|\vec{d}\}) = 0$ whenever $E_{nk} \neq E_{m\bar{g}k}$

$\Rightarrow$ if there is a state $|\psi_{nk}\rangle$ w/ energy E_{nk} there is another state $U_{\{\bar{g}|\vec{d}\}}|\psi_{nk}\rangle$ w/ energy

$$E_{n\bar{g}k} = E_{nk}$$



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

for $\vec{b} \in \check{T}$ a reciprocal lattice vector

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

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

Some Hilbert space

$$\Rightarrow \quad B^{k}_{ab}(\{\bar{g}|\vec{d}\}) := \langle \varphi_{a\bar{g}k} | U_{\{\bar{g}|\vec{d}\}} | \varphi_{bk} \rangle$$

is a map from a vector space to ~~itself~~ itself

Given some $\vec{k}_*$ we define $G_{k_*} < G$

$$G_{k_*} = \{ \{\bar{g}|\vec{d}\} \in G \mid \bar{g}k_* = k_* \text{ modulo } T \}$$

$\boxed{\text{little group of } k_*}$

$$\{ B^{k_*}_{ab}(g_*) \mid g_* \in G_k \} \leftarrow \text{forms a representation}$$

of G_k

Band basis: $|\psi_{nk_*}\rangle$

$$H|\psi_{nk_*}\rangle = E_{nk_*}|\psi_{nk_*}\rangle$$

$$H\,U_{g_*}|\psi_{nk_*}\rangle = E_{nk_*}\,U_{g_*}|\psi_{nk_*}\rangle$$

$$0 = \langle \varphi_{ak_*}|[H, U_{g_*}]|\varphi_{bk_*}\rangle$$

$$= \sum_c \langle \varphi_{ak_*}|H|\varphi_{ck_*}\rangle B^{k_*}_{cb}(g_*)$$

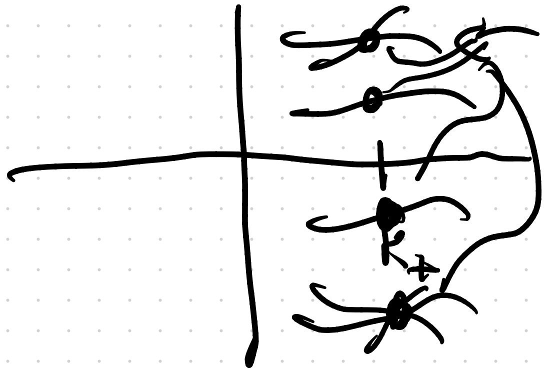
$$= \sum_c B^{k_*}_{ac}(g_*) \langle \varphi_{c k_*} | H | \varphi_{b k_*} \rangle$$

$$\Rightarrow [B^{k_*}(g_*), h(k_*)] = 0$$

we can label eigenstates of H by irreducible representations of the little group

$$B^{k_*}(g_*) \cong \bigoplus_i \eta_i^{k_*}$$

$\eta_i^{k_*}$ – little group irreps



transform in irreps of the little group

→ if there are little group irreps with dimension > 1 we have symmetry protected degeneracies