

Lecture 12 | • Make up lecture - Let's plan to stay an extra 1.5 hrs on 3/11 to catch up

Today: let's find $\tilde{h}(gk)$ in a particular case

Space group $P23$ (195)
Symmorphic \downarrow point 23 - tetrahedral symmetry
 $\leftarrow \langle C_{2z}, C_{3,111} \rangle$ cubic
Primitive cubic Bravais lattice

$$\vec{e}_1 = a\hat{x}$$

$$\vec{e}_2 = a\hat{y}$$

$$\vec{e}_3 = a\hat{z}$$

Let's look at states near the Γ point $(0,0,0)$

- $e_{\Gamma}(|E| \vec{r}) = e^{i\vec{k} \cdot \vec{r}} \rightarrow \text{identity } (1)$

- Irreps of G_{Γ} coincide with irreps of $23 = \overline{G}$

Irreps of \overline{G}

	E	C ₂	C ₃	C ₆ ⁻¹
Γ ₁	1	1	1	1
Γ ₂	1	1	e ^{2πi/3}	e ^{-2πi/3}
Γ ₃	1	1	e ^{-2πi/3}	e ^{2πi/3}
Γ ₄	3	-1	0	0

two dimensional real representation
("physically irreducible")

$$\text{tr}(\Gamma_{\psi}(E)) = 3$$

$$\Downarrow$$

$$\Gamma_4(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

3D vector representation of 2,3:

$$E: \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$\chi(E) = 3$$

lets consider p-orbitals in
p_z near Γ

$$C_{2v}: \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad \chi(C_{2v}) = -1$$

$$C_{3v}: \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} y \\ z \\ x \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad \chi(C_{3v}) = 0$$

to check that this is Γ_4 look at characters

✓✓

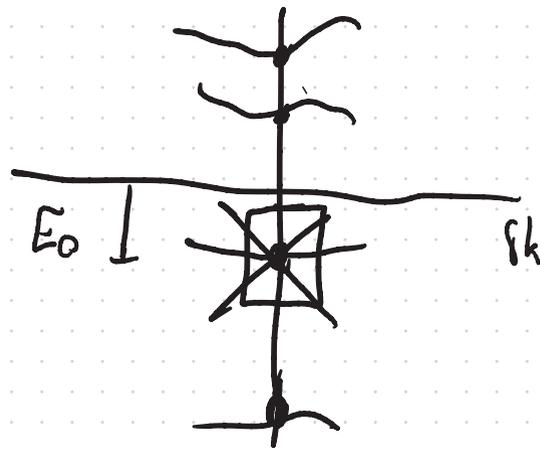
p -orbitals transform like vectors
($l=1$)

At Γ the hamiltonian $\hat{h}(\theta)$ is

the basis of p -orbitals reads

$$\tilde{h}(0) = E_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

What about $\tilde{h}(\delta k)$?



$$\Gamma_4(g)^\dagger \tilde{h}(\delta k) \Gamma_4(g) = \tilde{h}(g^{-1} \delta k)$$

$$\Gamma_4(g)^\dagger \tilde{h}(g \delta k) \Gamma_4(g) = \tilde{h}(\delta k)$$

Two constraint equations

$$C_{2,2} : \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \bar{h}(\delta k_x, \delta k_y, \delta k_z) \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix} = \bar{h}(\delta k_x, \delta k_y, \delta k_z)$$

$$C_{3,11} : \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \bar{h}(\delta k_y, \delta k_z, \delta k_x) \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = \bar{h}(\delta k_x, \delta k_y, \delta k_z)$$

To solve these eqns, lets introduce a basis for the space of 3×3 hamiltonians -

Gell-Mann matrices

$$9 \begin{pmatrix} \textcircled{0} & \textcircled{0} & \textcircled{0} \\ \vdots & \textcircled{0} & \textcircled{0} \\ \vdots & \vdots & \textcircled{0} \end{pmatrix} \text{ total matrices}$$

$$\lambda_0 = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix} \quad \lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_2 = \begin{pmatrix} 0 & & i \\ & i & \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_3 = \begin{pmatrix} 1 & & \\ & -1 & \\ & & 0 \end{pmatrix} \quad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

$$\lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & i & 0 \end{pmatrix} \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & & \\ & 1 & \\ & & -2 \end{pmatrix}$$

Consider the set $(\lambda_7, \lambda_5, \lambda_2)$

$$C_{\lambda_7} \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix} = - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & -i & 0 \end{pmatrix} = -\lambda_7$$

$$\Gamma_4(C_{2t})^\dagger \lambda_5 \Gamma_4(C_{2t}) = -\lambda_5$$

$$\Gamma_4(C_{2t})^\dagger \lambda_2 \Gamma_4(C_{2t}) = \lambda_2$$

$$C_{3,III} \quad \Gamma_4(C_{3,III})^\dagger \lambda_7 \Gamma_4(C_{3,III}) =$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & i & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -i \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} = -\lambda_5$$

$$\Gamma_4(C_{3111})^{\dagger} \lambda_5 \Gamma_4(C_{3111}) = \lambda_2$$

$$\Gamma_4(C_{3111}) \lambda_2 \Gamma_4(C_{3111}) = \lambda_7$$

$$\Gamma_4(C_{3111})^{\dagger} \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \Gamma_4(C_{3111}) = \begin{pmatrix} \lambda_5 \\ \lambda_2 \\ \lambda_7 \end{pmatrix}$$

$$\Gamma_4(C_{222})^{\dagger} \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \Gamma_4(C_{222}) = \begin{pmatrix} -\lambda_7 \\ -\lambda_5 \\ \lambda_7 \end{pmatrix}$$

The same thing is true of $\begin{pmatrix} \lambda_6 \\ \lambda_4 \\ \lambda_1 \end{pmatrix}$

$$(\delta k_x \quad \delta k_y \quad \delta k_z)$$

$$(\lambda_7, \lambda_5, \lambda_2)$$

$$(\lambda_6, \lambda_4, \lambda_1)$$

$\lambda_7 \delta k_x + \lambda_5 \delta k_y + \lambda_2 \delta k_z$ - solves my constraint eqns

$$\lambda_6 \delta k_x + \lambda_4 \delta k_y + \lambda_1 \delta k_z$$

To linear order in δk , these are the only solutions to our constraint eqns

$$\begin{aligned}\tilde{h}(\delta k) &= E_0 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + a(\lambda_7 \delta k_x + \lambda_5 \delta k_y + \lambda_2 \delta k_z) \\ &\quad + b(\lambda_6 \delta k_x + \lambda_4 \delta k_y + \lambda_1 \delta k_z)\end{aligned}$$

=

$$\begin{pmatrix} E_0 & c\delta k_z & c^*\delta k_y \\ c^*\delta k_z & E_0 & c\delta k_x \\ c\delta k_y & c^*\delta k_x & E_0 \end{pmatrix}$$

$$c = a - ib$$

$$+ O(\delta k^2)$$

$$\Gamma_4(C_{3111})^\dagger \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \Gamma_4(C_{3111}) = \begin{pmatrix} \lambda_5 \\ \lambda_2 \\ \lambda_7 \end{pmatrix} = \eta(C_{3111}) \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix}$$

$$\Gamma_4(C_{22})^\dagger \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \Gamma_4(C_{22}) = \begin{pmatrix} -\lambda_7 \\ -\lambda_5 \\ \lambda_7 \end{pmatrix} = \eta(C_{22}) \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix}$$

Claim: η defines a representation of \bar{G}

$$\Gamma_4(g_1 g_2)^t \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \Gamma_4(g_1 g_2) =$$

$$\begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \eta(g_1 g_2)$$

$$\Gamma_4(g_2)^t \left[\Gamma_4(g_1)^t \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \Gamma_4(g_1) \right] \Gamma_4(g_2)$$

$$\Gamma_4(g_2)^t \begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \eta(g_1) \Gamma_4(g_2)$$

$$\begin{pmatrix} \lambda_7 \\ \lambda_5 \\ \lambda_2 \end{pmatrix} \eta(g_2) \eta(g_1)$$

Now: going from little group representations
to space group irreps

To do so, we need to introduce a construction
called induction

Space group G , let's pick some \vec{k} and
look @ its little grp G_k

$$G_k \subset G$$

We can write a coset decomposition

$$G = \bigcup_{i=1}^N g_i G_k \quad (g_1 = E) \quad g_{i \neq 1} \notin G_k$$

Given a representation ρ_k of G_k , we
we will construct a representation of G

First say that $\rho_k: G_k \rightarrow U(V)$
(a representation on V)

$$W = \bigoplus_{i=1}^N V_i$$

I want a way to think
of V_i as $\mathcal{H}(g) V \rightarrow V_i$

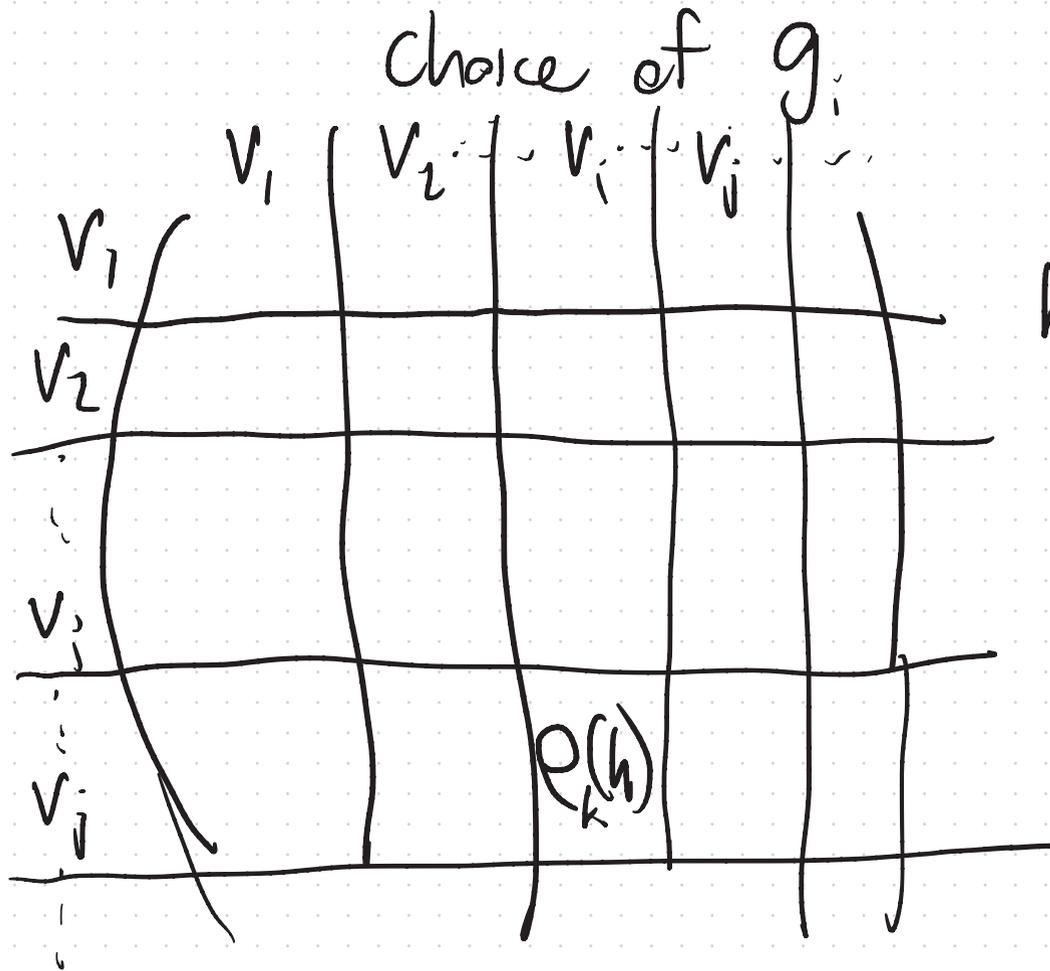
For any $g \in G$ and any fixed g_j
we know that $g g_j \in g_j G_k$

$$g g_j = g_j h \quad h \in G_k$$

$$g = g_j h g_j^{-1}$$

we can do this for each

$$\eta(g) =$$



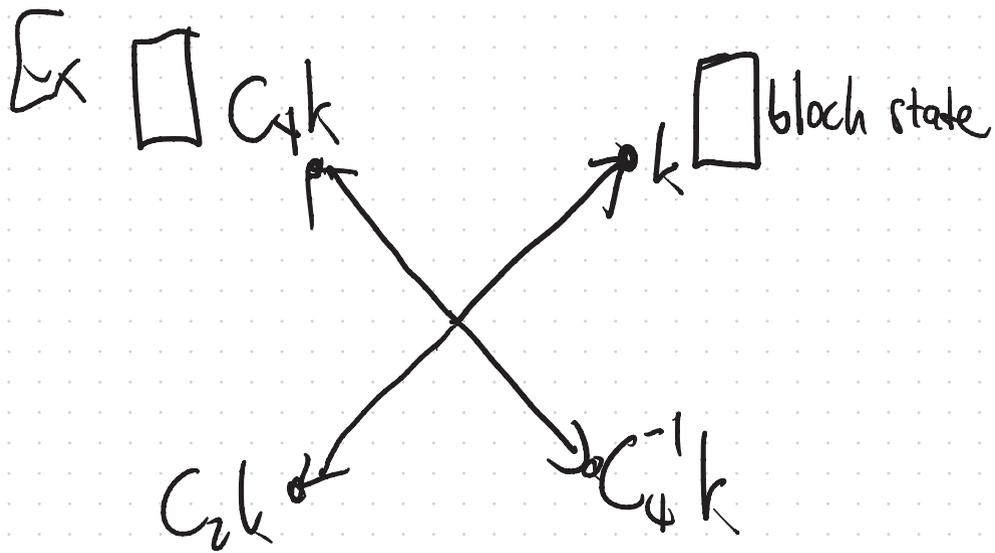
$$h = g_i g_j$$

For the little group, $V_{\vec{k}}$ is some space
of Bloch functions w/ wavevector \vec{k}

$$g \in G_{\vec{k}} \quad g \cdot \vec{k} \neq \vec{k}$$

$V_i =$ a space of Bloch functions at
 $g_i \cdot \vec{k}$

$\{g_i \cdot \vec{k} \mid i=1, \dots, N\}$ the star of \vec{k}



η is the representation of G induced from ρ_k

$$\begin{aligned}
 \eta &= \rho_k \hat{\uparrow} G \\
 &= \text{Ind}_{G_k}^G \rho_k
 \end{aligned}$$

$$\dim \mathfrak{g} = \dim \mathfrak{P}_k [G:G_k]$$