# Lecture 5

Announcement: Bravais lattices & compatible pt groups are on en.wikipedia.org/wiki/Crystal_system

- Recap: $H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$

$H = \frac{p^2}{2m} + V(\vec{r})$ $V(\vec{r})$ is invariant under the symmetries of a space grp $G$ w/ Bravais lattice $T$

$\forall \vec{t} \in T$ $U_{\vec{t}}|\psi_{nk}\rangle = e^{-i\vec{k}\cdot\vec{t}}|\psi_{nk}\rangle$

$\vec{k} \in$ 1st Brillouin zone

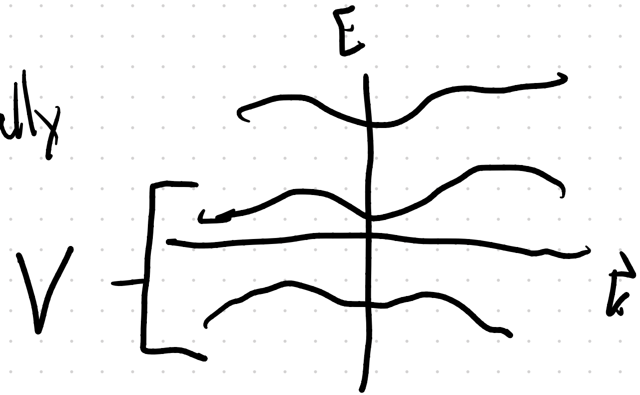
Representation $\rho$ of a group $G$ on some vector space $V$ s.t.

$\rho: G \to U(V)$

Some subspace of Bloch states $\{|\psi_{nk}\rangle\}$

$$\rho(g_1)\rho(g_2) = \rho(g_1 g_2)$$

Schematically




Example of a representation: $\vec{G} \in T$ Bravais lattice translations

$$V = \{|\psi_{nk}\rangle, n = 1, 2, \ldots N\}$$

$$\rho_k(\vec{t}) = U_{\vec{t}} = e^{-i\vec{k}\cdot\vec{t}}\,\delta_{nm}$$

$$U_{\vec{t}}\,|\psi_{n\vec{k}}\rangle = e^{-i\vec{k}\cdot\vec{t}}\,|\psi_{nk}\rangle = \sum_m \underbrace{e^{-i\vec{k}\cdot\vec{t}}\,\delta_{nm}}_{\rho(\vec{t})}\,|\psi_{mk}\rangle$$

$$\rho_k(\vec{t}_1+\vec{t}_2) = e^{-i\vec{k}\cdot(\vec{t}_1+\vec{t}_2)}\,\delta_{nm}$$

$$= \sum_l e^{-i\vec{k}\cdot\vec{t}}\,\delta_{nl}\; e^{-i\vec{k}\cdot\vec{t}_2}\,\delta_{lm} = \rho_k(\vec{t}_1)\,\rho_k(\vec{t}_2)$$

Q: is $\rho_k$ reducible or irreducible?

$$\rho_k(\vec{t}) = \left(\begin{array}{c|ccccc} 1 & & & & & \\ \hline & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{array}\right) e^{-i\vec{k}\cdot\vec{t}}$$

$|\psi_{nk}\rangle$ is an invariant subspace for each $n$

$$\rho_k(\vec{t})|\psi_{nk}\rangle \propto |\psi_{nk}\rangle$$

the irreducible rep is just $e^{-ik\cdot\vec{t}}(1)$

1x1 identity matrix

Schur's Lemma: Lets take a group $G$, and two irreducible representations $\rho_1 : G \to U(V_1)$

$\rho_2 : G \to U(V_2)$

If we have a linear map (matrix) $A : V_1 \to V_2$ such that $A\rho_1(g) = \rho_2(g)A \quad \forall g \in G$

Then either $A$ is invertible or $A = 0$

pf: lets consider $K = \{v \in V_1 \mid Av_1 = 0\}$

suppose $w \in K$ $w \neq 0$

$$A\rho_1(g)w = \rho_2(g)Aw = 0 \quad \text{forall } g\in G,\ w\in K$$

but this means $\rho_1(g)K \subset K$ for all $g\in G$

$\rightarrow$ $K$ is an invariant subspace of $\rho_1$

repeat same argument for image

$\rightarrow$ since $\rho_1$ is irreducible either $K = \emptyset \rightarrow A$ is invertible

$K = V_1 \rightarrow A = 0$

Corrolary: Suppose that $\rho_1 = \rho_2$ then $[A, \rho_1(g)]$

$\Rightarrow A = \lambda\, \mathrm{Id}$

pf: $A$ is a square matrix, so it has an eigenvalue

$\lambda$ and an eigenvector $v$

s.t. $Av = \lambda v$

$B = A - \lambda \, \mathrm{Id}$

$Bv = 0$ and $[B, \rho_1(g)] = 0 \; \forall g$

$\rightarrow$ Schurs lemma $\Rightarrow B = 0$

$\rightarrow A = \lambda \, \mathrm{Id}$

What does this corrolary mean for QM:

$H|\psi_i\rangle = E_i |\psi_i\rangle$ if we have some

group $G$ of symmetries then lets consider

$\{|\psi_i\rangle\}$ a subset of Bloch states that transform in a irreducible representation (irrep) $\rho$ of $G$

$$U_g|\psi_i\rangle = \sum_j |\psi_j\rangle \rho_{ji}(g)$$

$$U_g^\dagger H U_g = H$$

$$[H]_{ij} = \langle\psi_i|H|\psi_j\rangle$$
$$= \langle\psi_i|U_g^\dagger H U_g|\psi_j\rangle$$

$$= \sum_{k\ell} \rho^\dagger_{ik}(g) [H]_{k\ell} \rho_{\ell j}(g)$$

$$[[H], \rho(g)] = 0$$

$$\rightarrow [H]_{ij} = E\,\delta_{ij}$$ by Schur's lemma

$$\boxed{\text{states that transform in irreps of } G \text{ are degenerate}}$$

if we can find irreps of space groups, then we can know about symmetry-enforced degeneracies between Bloch States.

<u>Character theory</u>: We can characterize representations by looking at traces of matrices

<u>Def</u> $\chi_\rho$ ← the character of representation $\rho$ of grp $G$

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

Some important properties of characters:

① $\chi_\rho(g_1 g_2 g_1^{-1}) = \mathrm{tr}\,\rho(g_1 g_2 g_1^{-1})$

$$= \mathrm{tr}\left[\rho(g_1)\rho(g_2)\rho(g_1^{-1})\right]$$

$$= \mathrm{tr}\left[\rho(g_1^{-1})\rho(g_1)\rho(g_2)\right]$$

$$= \mathrm{tr}\left[\rho(g_2)\right]$$

$$= \chi_\rho(g_2)$$

Conjugacy class $C(g) = \{hgh^{-1} \mid h \in G\}$

Characters are constant on conjugacy classes

(2) $\rho_3 = \rho_1 \oplus \rho_2$ i.e. $\rho_3(g) = \begin{pmatrix} \rho_1(g) & 0 \\ 0 & \rho_2(g) \end{pmatrix}$

$$\chi_{\rho_3}(g) = \mathrm{tr}\left[\rho_3(g)\right] = \mathrm{tr}\left[\begin{pmatrix} \rho_1(g) & 0 \\ 0 & \rho_2(g) \end{pmatrix}\right]$$

$$= \mathrm{tr}\,\rho_1(g) + \mathrm{tr}\,\rho_2(g)$$

$$= \chi_{\rho_1}(g) + \chi_{\rho_2}(g)$$

$$\chi_{\rho_1 \oplus \rho_2} = \chi_{\rho_1} + \chi_{\rho_2}$$

3 if $\rho_1$ and $\rho_2$ are isomorphic in the sense that

$U\rho_1(g)U^\dagger = \rho_2(g)$ then $\chi_{\rho_1} = \chi_{\rho_2}$

Lets do a quick example

pt group 6mm $\quad G = \langle C_{6z}, M_x \rangle$

Lets look at two representations:

① Trivial representation $\rho_0 \quad \rho_0(C_6) = \mathbb{1} = \rho_0(M_x)$

$$\chi_{\rho_0}(g) = tr(\rho_0(g)) = tr(\mathbb{1}) = 1$$

② Vector representation $\left\{ \begin{pmatrix} x \\ y \end{pmatrix} \right\} = V$

$$\rho_V(C_6) = \begin{pmatrix} \cos\frac{2\pi}{6} & \sin\frac{2\pi}{6} \\ -\sin\frac{2\pi}{6} & \cos\frac{2\pi}{6} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

$$\rho_V(m_x) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\chi_{\rho_V}(C_6) = tr\left[\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}\right] = \frac{1}{2} + \frac{1}{2} = 1$$

$$\chi_{\rho_V}(m_x) = tr\left[\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}\right] = 0$$

Theres another 2d rep I can write

$$\rho'(m_x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\rho'(C_6) = \begin{pmatrix} e^{2\pi i/3} & 0 \\ 0 & e^{-2\pi i/3} \end{pmatrix}$$

$$\chi_{\rho'}(M_x) = 0$$

$$\chi_{\rho'}(C_6) = 2\cos\frac{2\pi}{3} = -1$$

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We are going to show that characters for irreducible representations form a basis for the set of all characters.

Suppose we have two irreps $\rho_1, \rho_2$ of $G$

$\rho_1 : G \to U(V_1)$

$\rho_2 : G \to U(V_2)$

and some we have some $A : V_1 \to V_2$ but

$A$ might not commute w/ the action $\rho_1, \rho_2$

$$A\rho_1(g) \neq \rho_2(g)A$$

We can always construct

$$A_G = \sum_{g \in G} \rho_2(g^{-1}) A \rho_1(g)$$

then $$A_G \rho_1(g') = \sum_{g \in G} \rho_2(g^{-1}) A \rho_1(g) \rho_1(g')$$

$$= \sum_{g \in G} \rho_2(g^{-1}) A \rho(gg')$$

$$g'' = gg'$$

$$g = g'' g'^{-1}$$

$$g^{-1} = g'(g'')^{-1}$$

$$= \sum_{g'' \in G} \rho_2(g'(g'')^{-1}) A \rho(g'')$$

$$= \rho_2(g') \sum_{g'' \in G} \rho((g'')^{-1}) A \rho(g'')$$

$$= \rho_2(g') A_G$$

$\Rightarrow$ $A_G$ is either invertible or zero

$$\rho_1 = \rho_2$$

and $A_0 = \lambda \mathrm{Id}$

Lets see what happens when $A$ is equal to a matrix with only one nonzero entry

$$A = E_{\underset{V_2}{i_2}\,\underset{V_1}{j_1}} = \begin{array}{cl} \begin{pmatrix} & & & & \\ & & 1 & & \\ & & & & \\ & & & & \end{pmatrix} & i_2\text{-th row} \\ j_1\text{-th column} & \end{array}$$

$$A_G = \left(E_{i_2 j_1}\right)_G = \sum_{g \in G} \rho_2(g^{-1}) E_{i_2 j_1} \rho_1(g)$$

$$[A_G]^{k\ell} = \sum_{g \in G} \left[\rho_2(g^{-1})\right]^{k i_2} \left[\rho_1(g)\right]^{j_1 \ell}$$

$$= \begin{cases} 0 & \text{if } \rho_1 \neq \rho_2 \\ \lambda \delta_{k\ell} & \text{if } \rho_1 = \rho_2 \end{cases}$$