Lecture 6

- HW 2 will be posted 9/19
- Making up lost lecture: 9/19, 9/21 extended by 40 mins

Recap: Characters of representations

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

Character of ρ $\quad \chi_\rho : G \to \mathbb{C}$

$\chi_\rho(g) = tr(\rho(g))$

Schur Orthogonality Relations:

if we have two irreps ρ_1, ρ_2 of G

$$\sum_{g\in G} [\rho_2(g^{-1})]_{\alpha\mu} [\rho_1(g)]_{\nu\beta} = \begin{cases} 0 & \text{if } \rho_1 \neq \rho_2 \\ \frac{|G|}{\dim \rho_1} \delta_{\mu\nu} \delta_{\alpha\beta} & \text{if } \rho_1 = \rho_2 \end{cases}$$

equal- same basis

lets us define an inner product on characters

$$\langle \chi_1, \chi_2 \rangle = \frac{1}{|G|} \sum_{g\in G} \chi_1^*(g) \chi_2(g) = \frac{1}{|G|} \sum_{g\in G} \chi_1(g^{-1}) \chi_2(g)$$

if ρ_1 and ρ_2 are irreducible, then

$$\langle \chi_{\rho_1}, \chi_{\rho_2} \rangle = \begin{cases} 0 & \text{if } \rho_1 \neq \rho_2 \\ 1 & \text{if } \rho_1 \simeq \rho_2 \end{cases}$$

equivalent up to a basis transformation

[unitarity $\rho^\dagger(g) = \rho(g^{-1})$]

Two final points about characters:

- The irreducible characters form a complete basis for functions invariant under conjugation.

Given *any* function $f : G \to \mathbb{C}$

$f(h) = f(ghg^{-1})$ for all g and h

└ Class function

We have $f = \sum_{\substack{\text{irreps} \\ e_n}} \alpha_{e_n} \chi_{e_n}$ $\quad \alpha_{e_n} \in \mathbb{C}$

$\Rightarrow$ # of irreps of a group = # of conjugacy classes

Conjugacy class:

$g \in G$

$C_g = \{ g' g g'^{-1} \mid g' \in G \}$

If G has N conjugacy classes

$G = C_1 \cup C_2 \cup \cdots \cup C_N$

Then $f_n(g) = \begin{cases} 1 & \text{if } g \in C_n \\ 0 & \text{otherwise} \end{cases}$

there's N of $f_n \Rightarrow$ there must be N irreducible characters

To prove this, procede by contradiction

suppose $f: G \to \mathbb{C}$ is a class function, and suppose that

$\langle \chi_{\rho_i}, f \rangle = 0$ for all irreps ρ_i

then $f = 0$

$$f_i = \sum_{g \in G} f(g^{-1}) \rho_i(g)$$

this is a matrix b/c ρ_i is a matrix and $\rho_i(g') f_i = \sum_{g\in G} f(g^{-1}) \rho_i(g') \rho_i(g)$

$$= \sum_{g\in G} f(g^{-1}) \rho_i(g'g)$$

$$= \sum_{g''\in G} f(g'^{-1} g''^{-1} g') \rho_i(g'' g')$$

$$= \left[\sum_{g''\in G} f(g'')^{-1} \rho_i(g'')\right] \rho_i(g')$$

$$= f_i \rho_i(g')$$

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

$$g'g = g''g'$$

$$g^{-1} = \left[g'^{-1} g'' g'\right]^{-1}$$

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

$[f_i, \rho_i(g')] = 0 \Rightarrow f_i = \lambda\, Id$ by Schur's lemma to find λ, take traces

$$\mathrm{tr}\left[\sum_{g\in G} f(g^{-1})\rho_i(g)\right] = \lambda\,\mathrm{tr}(\mathrm{Id}) = \lambda \dim\rho_i$$

$$= \sum_{g\in G} f(g^{-1})\chi_{\rho_i}(g) = \lambda \dim\rho_i$$

$$= |G|\langle f, \chi_{\rho_i}\rangle = 0 \Rightarrow \lambda = 0 \Rightarrow f_i = 0$$

To use this to prove that $f=0$, we can construct a representation called the <u>regular representation</u>

$$\rho_{reg} : G \to U(\mathbb{C}^{|G|})$$

Basis vectors $\{\vec{e}_g, g\in G\}$ $\quad \vec{e}_g\cdot\vec{e}_{g'} = \delta_{gg'}$

$$\rho_{reg}(g)\vec{e}_{g'} = \vec{e}_{gg'}$$

$$[\rho_{reg}(g)]_{hg'} = \begin{cases} 1 & \text{if } h = gg' \\ 0 & \text{otherwise} \end{cases}$$

ρ_{reg} is some sum of irreducible representations

$$\Rightarrow \langle f, \chi_{\rho_{reg}} \rangle = 0$$

$$\tilde{f} = \sum_{g \in G} f(g^{-1})\rho_{reg}(g) \qquad \tilde{f} = 0 \text{ by Schur's lemma}$$

$$\tilde{f}\vec{e}_E = \sum_{g \in G} f(g^{-1})\rho_{reg}(g)\vec{e}_E$$

$$= \sum_{g \in G} f(g^{-1}) \vec{e}_g = 0$$

$$\Rightarrow f(g^{-1}) = 0 \text{ for all } g$$

→ the irreducible characters span the space of class functions

→ the # of irreps of a group = the # of conjugacy classes in the group

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Using Schur's lemma, we can use characters to find explicit projectors onto invariant subspaces

Given a reducible representation

$$\eta = \bigoplus_i n_i \rho_i$$

$\uparrow$ multiplicity of ρ_i in η

ρ_i irreducible

$n_i \rho_i$ is shorthand for $\underbrace{\rho_i \oplus \rho_i \oplus \cdots \oplus \rho_i}_{n_i \text{ times}}$

is a representation on a vector space

$$V = \bigoplus_i V_i^{n_i}$$

we want to find matrices P_i s.t.

$$P_i \vec{u} = \begin{cases} \vec{u} & \text{if } \vec{u} \in V_i \\ 0 & \text{otherwise} \end{cases}$$

(from Schur's lemma, Hamiltonians are block-diagonal in the V_i's)

Taking inspiration from our previous proof:

$$P_i = \frac{\dim \rho_i}{|G|} \sum_{g \in G} \chi_{\rho_i}(g^{-1}) \, \eta(g)$$

In our basis where η is block-diagonal

$$[P_i]^{ab} = \frac{\dim \rho_i}{|G|} \sum_{g \in G} \chi_{\rho_i}(g^{-1}) \bigoplus_j \rho_j^{ab}(g)$$

$$= \frac{\dim \rho_i}{|G|} \sum_{g \in G} \bigoplus_j \sum_c \rho_i^{cc}(g^{-1}) \rho_j^{ab}(g)$$

$$= \frac{\cancel{\dim \rho_i}}{\cancel{|G|}} \sum_c \bigoplus_j \left(\frac{\cancel{|G|}}{\cancel{\dim \rho_i}} \right) \delta_{ij} \delta_{ac} \delta_{bc}$$

$$= \bigoplus_j \delta_{ij} \delta_{ab} \Rightarrow P_i \text{ projects onto the irreducible representation } \rho_i$$

With the group theory done, lets turn back to Physics;

Lets look at electrons in solids (ignoring interactions for now)

ionic potential $V(\vec{x})$

Hamiltonian $H = \frac{p^2}{2M} + V(\vec{x})$

Symmetries of H are a subgroup of $\mathbb{E}(3) = \mathbb{R}^3 \rtimes O(3)$

translations in 3D, rotations and reflections

$$V(g\,\vec{x}) = V(\vec{x})$$

the group G of rigid symmetries of a 3D crystal is called a <u>Space group</u> $G \subset \mathbb{E}(3)$

The key thing that defines a crystal is discrete translation symmetry: Every space group G has a subgroup

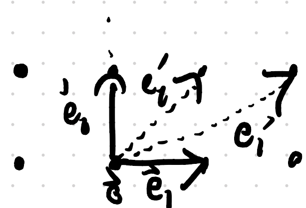
$$T = \left\{ \{E \,|\, n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3\},\ n_i \in \mathbb{Z} \right\}$$

T - the Bravais lattice of the space group

$\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ - primitive lattice vectors (not unique)

$$V(\vec{x} + n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3) = V(\vec{x})$$

Ex: 2D



$\vec{e}_1 = (a, 0)$

$\vec{e}_2 = (0, a)$