# Lecture 6

Recap: $\rho : G \to U(V)$ a (finite dimensional) representation of $G$

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

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

- Characters are constant on conjugacy classes (class functions)

Schur Orthogonality Relations: if $\rho_1, \rho_2$ are irreps:

(1) $$\sum_{g\in G} [\rho_2(g^{-1})]^{\mu i} [\rho_1(g)]^{j\nu} = \begin{cases} 0, & \rho_1 \not\cong \rho_2 \\ \frac{|G|}{\dim \rho_1} \delta_{ij}\delta_{\mu\nu}, & \rho_1 = \rho_2 \end{cases}$$

(2) $$\underbrace{\frac{1}{|G|}\sum_{g\in G} \chi^*_{\rho_2}(g)\chi_{\rho_1}(g)}_{\langle \chi_{\rho_2}, \chi_{\rho_1}\rangle} = \begin{cases} 0 & \text{if } \rho_1 \not\cong \rho_2 \\ 1 & \text{if } \rho_1 \cong \rho_2 \end{cases} \text{ "}\delta_{\rho_1\rho_2}\text{"}$$

$\leftarrow$ Characters of irreducible representations are orthonormal under $\langle , \rangle$

$\rightarrow$ Corollary! Characters are class functions $\rightarrow$ number of irreducible characters $\leq$

number of conjugacy classes of the group

Ex: $D_2 = \{E, C_{2x}, C_{2y}, C_{2z}\}$

irreps

| | $E$ | $C_{2x}$ | $C_{2y}$ | $C_{2z}$ |
|---|---|---|---|---|
| $B_1$ | 1 | 1 | -1 | -1 |
| $B_2$ | 1 | -1 | 1 | -1 |
| $B_3$ | 1 | -1 | -1 | 1 |
| $A$ | 1 | 1 | 1 | 1 |

Character table

Conjugacy classes

trivial representation $\to$ A

Final point: # of distinct irreps = # of conjugacy classes of the group

→ irreducible characters form an orthonormal

# basis for class functions

To see this let's define the <u>regular representation</u>

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

$\mathbb{C}^{|G|}$ : Basis vectors $\{\vec{e}_g \mid g \in G\}$ $\quad \vec{e}_{g_i} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{pmatrix} \downarrow i$

$$\langle \vec{e}_{g_i}, \vec{e}_{g_j} \rangle = \vec{e}_{g_i}^{\dagger} \cdot \vec{e}_{g_j} = \delta_{ij}$$

$$\rho_{reg}(g)\vec{e}_{g_i} = \vec{e}_{gg_i}$$

$$[\rho_{reg}(g)]_{ij} = \vec{e}_{g_i}^{\,t} \cdot \rho(g) \cdot \vec{e}_{g_j} = \vec{e}_{g_i}^{\,t} \cdot \vec{e}_{gg_j} = \begin{cases} 1 & \text{if } g_i = gg_j \\ 0 & \text{otherwise} \end{cases}$$

Now suppose $f$ is a class function $\langle \chi_{\rho_i}, f \rangle = \sum_{g \in G} \frac{1}{|G|} \overline{\chi}(g) f(g) = 0$

for all irreps $\rho_i$

Then $f = 0$

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

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

$$[f_i, \rho_i(g)] = 0$$

Schur's lemma pt 2: $f_i = \lambda \, \mathrm{Id}$

But $\operatorname{tr} f_i = \lambda \dim \rho_i$

$$\operatorname{tr} f_i = \sum_{g \in G} f(g^{-1}) \chi_{\rho_i}(g) = 0$$

so $\lambda = 0 \Rightarrow f_i = 0$

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

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

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

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

Since every rep is a sum of irreps

$$f_{reg} = \sum_{g \in G} f(g^{-1}) \rho_{reg}(g) = 0$$

$$0 = f_{reg}\vec{e}_E = \sum_{g\in G} f(g^{-1})\underbrace{\rho_{reg}(g)\vec{e}_E}$$

$$= \sum_{g\in G} f(g^{-1})\,\vec{e}_g = \begin{pmatrix} f(E) \\ f(g_1^{-1}) \\ f(g_2^{-1}) \\ \vdots \end{pmatrix} = 0$$

$\Rightarrow$ $f$ is zero on every group element

$\Rightarrow$ $f = 0$

$\Rightarrow$ irreducible characters span the space of class functions

$\Rightarrow$ # of irreducible reps = # of conjugacy classes

→ Character tables are square

$$
\text{irreps} \rightarrow
\begin{array}{c|cccc}
 & C_1 & C_2 & \cdots & C_n \\
\hline
\rho_1 & \chi_{\rho_1}(C_1) & \chi_{\rho_1}(C_2) & \cdots & \\
\rho_2 & \vdots & & & \\
\rho_3 & \vdots & & & \\
\vdots & & & &
\end{array}
\quad \leftarrow \text{conjugacy classes}
$$

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Turning to physics: Electrons in solids (ignore interactions)

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

$V(\vec{x})$ - external potential due to ions in a crystal

rigid symmetries of $H$ $\quad G < E(3) = \mathbb{R}^3 \rtimes O(3)$

$V(g^{-1}\vec{x}) = V(\vec{x})$ $\quad$ $g = \{\underbrace{R}_{O(3)} | \underbrace{\vec{d}}_{\mathbb{R}^3}\} \in G$ $\quad$ $g\vec{x} = [R]\vec{x} + \vec{d}$

The group of rigid symmetries of a crystal are called <u>space groups</u>

Defining feature of a crystal $\rightarrow$ discrete translation symmetry

Every space group $G$ has a subgroup

$$T = \{\{E | \sum_i n_i \vec{e}_i\} | n_i \in \mathbb{Z}\}$$

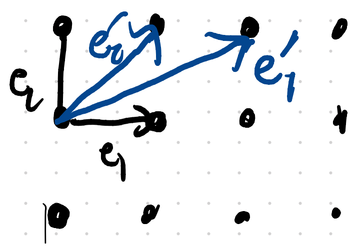
Bravais lattice

a set of linearly independent vectors : "primitive lattice vectors"

$T \triangleleft G$ is a normal subgraps

$$V\left(\vec{x} - \sum_i n_i \vec{e}_i\right) = V(\vec{x})$$

Ex 2D Bravais lattice $\vec{e}_1 = (a,0)$, $\vec{e}_2 = (0,a)$ $\quad T \ni n_1\vec{e}_1 + n_2\vec{e}_2$



**Primitive unit cell**: connected subspace of $\mathbb{R}^3$ s.t. no two points can be related by an element of $\overline{T}$

Lecture 2/3: $\mathbb{R}^3 / T$ - set of cosets of $T$ in $\mathbb{R}^3$

$$\rotatebox{90}{$\subset$}$$

$$\left\{ \left\{ E \,\middle|\, \sum_i n_i \vec{e}_i + \vec{v} \right\} \,\middle|\, \vec{v} \in \mathbb{R}^3,\ n_i \in \mathbb{Z} \right\}$$

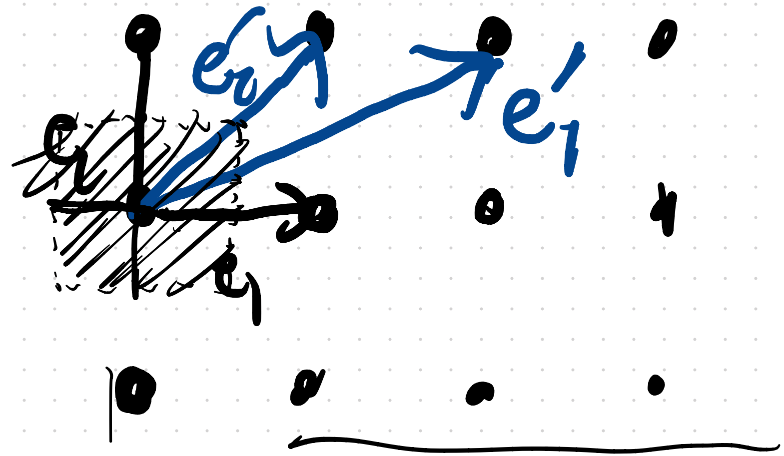
Concrete construction: given $\{\vec{e}_i\}$ primitive lattice vectors

$$\mathbb{R}^3 / T \simeq \left\{ \sum_i \alpha_i \vec{e}_i \,\middle|\, \alpha_i \in \left(-\tfrac{1}{2}, \tfrac{1}{2}\right] \right\}$$

$\alpha_i$: reduced coordinates

$(\alpha_1, \alpha_2, \alpha_3)$

2D




Lets look at how $T$ is represented an Hilbert space

$$T \ni \vec{t} = \sum_i n_i \vec{e}_i \longrightarrow e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{t}} = U_{\vec{t}} \in U(\mathcal{H})$$

$$\rho : T \to U(\mathcal{H})$$
$$\vec{t} \to U_{\vec{t}}$$

is a representation

$$\langle \vec{r} | U_{\vec{t}} | \psi \rangle = \psi(\vec{r} - \vec{t})$$

$$\boxed{\text{For abelian groups, all irreps are 1D}}$$

Abelian: $U_{t_1} U_{t_2} = U_{t_2} U_{\vec{t}_1} = U_{\vec{t}_1 + \vec{t}_2}$

$\to$ Can simultaneously diagonalize $U_{\vec{t}}$ for all $\vec{t} \in T$

$$U_{\vec{t}} = \begin{pmatrix} \lambda_1(\vec{t}) & & & \\ & \lambda_2(\vec{t}) & & \\ & & \lambda_3(\vec{t}) & \\ & & & \ddots \end{pmatrix}$$

$$U_{\vec{t}}|\varphi\rangle = \lambda_{\vec{t}}|\varphi\rangle \quad \text{for all } \vec{t} \in T$$

$\lambda_{\vec{t}}$ is a 1D irrep of $T$

$$\boxed{\begin{aligned} &\lambda_{\vec{0}} = 1 \quad \lambda_{\vec{t}_1}\lambda_{\vec{t}_2} = \lambda_{\vec{t}_1+\vec{t}_2} \\ &\lambda_{-\vec{t}} = \lambda_{\vec{t}}^{-1} \end{aligned}}$$

$$\lambda_{\vec{t}} = e^{-i\vec{k}\cdot\vec{t}}$$

These are the 1D irreps of $T$

$\vec{k}$ indexes these irreps, called crystal momentum

Hamiltonian is translation invariant: $[H, U_{\vec{t}}]$

$\langle \varphi_k | H | \varphi_{k'} \rangle = 0$ if $k$ and $k'$ are distinct irreps

we can diagonalise $H$ by first finding translation eigenstates

$$H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$$

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

← Bloch's theorem

$$\downarrow$$

$$\psi_{nk}(\vec{r}-\vec{t}) = \langle \vec{r} | U_{\vec{t}} | \psi_{nk} \rangle = e^{-i\vec{k}\cdot t}\, \psi_{nk}(\vec{r})$$

$$\psi_{nk}(\vec{r}) = e^{ik\cdot r}\, u_{nk}(r) \qquad u_{nk}(r-t) = u_{nk}(\vec{r})$$

What are the distinct irreps of $T$?

two irreps $k_1, k_2$

$$\vec{t} \to e^{-ik_1 \cdot \vec{t}}$$

$$\vec{t} \to e^{-ik_2 \cdot \vec{t}}$$

These are the same irrep if $e^{-ik_1 \cdot \vec{t}} = e^{-ik_2 \cdot \vec{t}}$ forall $\vec{t} \in T$

$$e^{i(k_1 - k_2) \cdot \vec{t}} = 1 \quad \text{for all } t \in T$$

$\Rightarrow (k_1 - k_2) \cdot \vec{t} = 2\pi n_{\vec{t}}$ $\quad n_{\vec{t}} \in \mathbb{Z}$

To solve this, introduce reciprocal lattice $\check{\Gamma}$

given $\{\vec{e}_i\}$ primitive Bravais lattice vectors

introduce primitive reciprocal lattice vectors

$\vec{b}_i : \quad \vec{b}_i \cdot \vec{e}_j = 2\pi \delta_{ij}$

$\Rightarrow \quad \vec{k}_1 - \vec{k}_2 = \sum_i m_i \vec{b}_i \in \check{\Gamma}$

Space of distinct irreps → primitive unit cell of $\check{T}$ ← Brillouin Zone

$$\left\{ \sum_i k_i \vec{b}_i \;\middle|\; k_i \in \left[-\tfrac{1}{2}, \tfrac{1}{2}\right] \right\}$$

reduced coordinates of $\vec{k}$