Lecture 6

Reminders: HW1 due 9/19

Office hrs Wednesdays 4-5pm

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

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

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

Schur Orthogonality Relations if ρ_1, ρ_2 are irreducible

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

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

$$\| $$

$$\langle \chi_{\rho_2},\chi_{\rho_1}\rangle$$

One final point: Irreducible characters form a complete basis for the space of class functions

→ # of distinct irreps of G = # of conjugacy classes of G

To see this lets introduce the <u>regular representation</u>

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

Basis vectors $\{\vec{e}_g \mid g \in G\}$ $\vec{e}_{g_i} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$ ← ith element

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

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

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

Pf: Let f be a class fn s.t. $\langle \chi_{\rho_i}, f \rangle = \sum_{g \in G} \chi_{\rho_i}^*(g) f(g) = 0$

for all irreps ρ if we show $f = 0$ then we're done

for each irrep ρ

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

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

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

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

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

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

→ Schur's lemma pt 2 $f_i = \lambda \, Id$

but $tr(f_i) = |G| \langle f, \chi_{\rho_i} \rangle = 0$

→ $f_i = 0$

This is true for every irrep → true for every sum of irreps ⇒

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

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

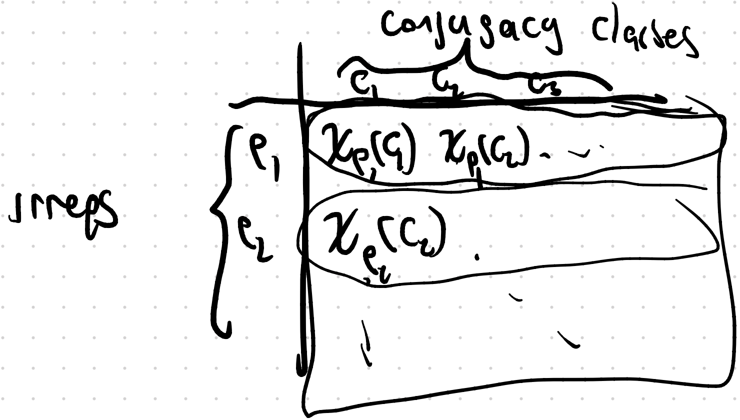
$$= \sum_{g\in G} f(g^{-1})\vec{e}_g = \begin{pmatrix} f(E) \\ f(g_1^{-1}) \\ f(g_2^{-1}) \\ f(g_3^{-1}) \\ \vdots \end{pmatrix} = 0$$

$$\Rightarrow f = 0$$

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

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

Last class - summarize irreps for a group in Character tables - Character tables are always square



← Character tables are unitary matrices

Turning to Physics: Electrons in Solids (ignore interactions for now)

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

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

Study group of symmetries $G \subset E(3) = \mathbb{R}^3 \rtimes O(3)$

$$g = \{R | \vec{d}\} \in G$$

$$V(g^{-1}\vec{x}) = V(\vec{x}) \qquad g = \{R|\vec{d}\} \qquad g\vec{x} = [R]\vec{x} + \vec{d}$$

The group of rigid symmetries of a crystal is called a <u>Space group</u>

Defining feature of a crystal: discrete translation symmetry

Every space group G has a subgroup

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

"primitive lattice vectors"
↓
$\vec{e}_i$ - linearly indep. vectors

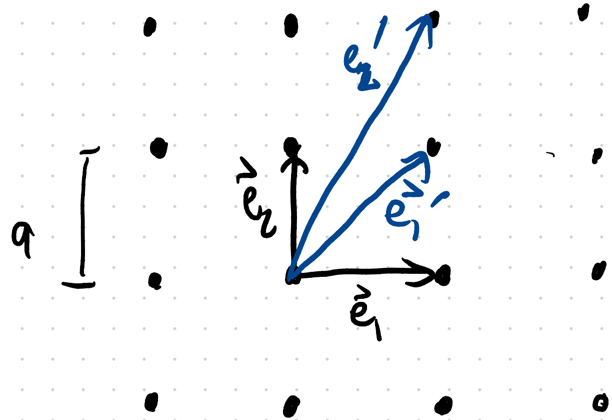
$T \triangleleft G$ - Bravais lattice of translations is a normal subgroup of a space group

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

Ex: 2D Bravais lattice

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

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



$$T \ni n_1 \vec{e}_1 + n_2 \vec{e}_2$$

$$\{R|\vec{d}\}\{E|\vec{v}\}\{R|\vec{d}\}^{-1} = \{E|R\vec{v}\}$$

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

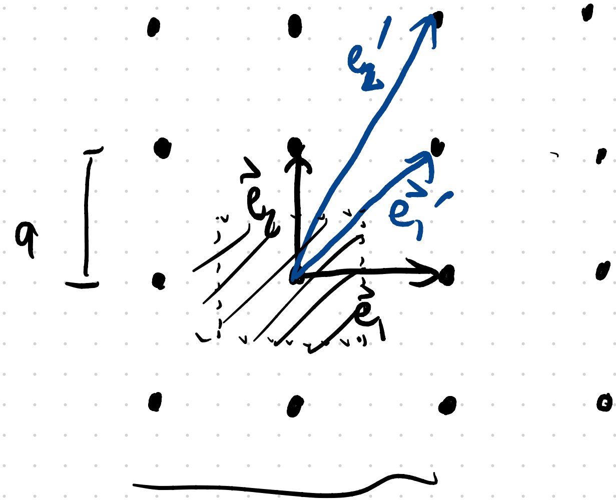
Lecture 2: $\mathbb{R}^3/T$ - Set of cosets of T in

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

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

$$\left\{ \sum_i \alpha_i \vec{e}_i \quad \alpha_i \in \left(-\tfrac{1}{2}, \tfrac{1}{2}\right] \right\}$$

$(\alpha_1, \alpha_2, \ldots)$ - Reduced coordinates



Lets look at how T is represented on quantum states

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

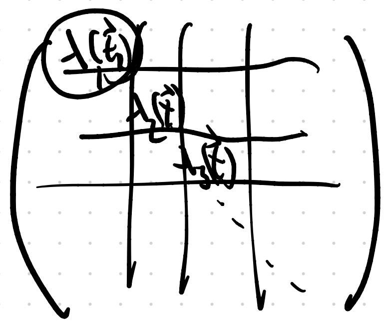
$$\langle \vec{r} | U_t | \psi \rangle = \psi(\vec{r} - \vec{t})$$

$\rho : \vec{t} \to U_{\vec{t}}$ is a representation of T

$$\begin{cases} U_{t_1}U_{t_2} = e^{-\frac{i}{\hbar}\vec{p}\cdot t_1} e^{-\frac{i}{\hbar}\vec{p}\cdot t_2} = e^{-\frac{i}{\hbar}\vec{p}\cdot (t_1+t_2)} = U_{t_1+t_2} \\ U_{t_1}U_{t_2} = U_{t_2}U_{t_1} \quad \text{abelian} \end{cases}$$

We can simultaneously diagonalize every $U_{\vec{t}}$ → find irreducible reps of T

$U_{\vec{t}} =$



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

↓

$\lambda_{\vec{0}} = 1 \qquad \lambda_{t_1+t_2} = \lambda_{t_1}\lambda_{t_2}$

$\lambda_{-\vec{t}} = \lambda_{\vec{t}}^{-1}$

$\Big\} \; e^{i\vec{k}\cdot\vec{t}}$

crystal momentum

$\vec{k}$ labels irreps of Bravais lattice T

$[H, U_{\vec{t}}] = 0$ for ever $\vec{t} \in T$

$\langle \psi_k | H | \psi_{k'} \rangle \propto \delta_{kk'}$ if $U_{\vec{t}}|\psi_{k'}\rangle = e^{-i\vec{t}\cdot k'}|\psi_{k'}\rangle$

$U_{\vec{t}}|\psi_k\rangle = e^{-i\vec{t}\cdot k}|\psi_k\rangle$

By Schur's lemma

$\rightarrow$ $H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle$ Bloch's theorem

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

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

$$e^{ik\cdot\vec{r}}\,u_{nk}(r) \longrightarrow u_{nk}(\vec{r}-\vec{t}) = u_{nk}(\vec{r}) \text{ periodic}$$

What are the distinct irreps of T?

two irreps $\vec{k}_1, \vec{k}_2$ are the same if $e^{-i\vec{k}_1\cdot\vec{t}} = e^{-i\vec{k}_2\cdot\vec{t}}$ $\forall \vec{t}$

$$(\vec{k}_1 - \vec{k}_2)\cdot\vec{t} = 2\pi\, n_{\vec{t}} \quad \forall \vec{t}$$

$(\vec{k}_1-\vec{k}_2)\cdot\vec{e}_i = 2\pi n_i$ for our primitive lattice vectors

to solve this, can introduce the <u>reciprocal lattice</u>

introduce $\vec{b}_i$ s.t. $\vec{b}_i\cdot\vec{e}_j = 2\pi\delta_{ij}$ primitive reciprocal lattice vectors

$$\vec{k}_1-\vec{k}_2 = \sum_i m_i \vec{b}_i \in \Upsilon = \left\{ \sum_i m_i \vec{b}_i \,\middle|\, m_i \in \mathbb{Z} \right\}$$

↑ reciprocal lattice

Space of distinct irreps → primitive unit cell in reciprocal lattice Brillouin zone (BZ)

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

k_i - reduced coordinates of $\vec{k}$