Lecture 6

Reminder: HW I is due Tuesday 2/6 on Gradescope

Recap: Representation $\rho : G \to U(V)$ of G on V

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

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

Schur Orthogonality relations: two irreducible representations ρ_1 and ρ_2 of G

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

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

$$\| $$

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

Characters are "class functions"

$$f(h) = f(ghg^{-1})$$

One final point about characters:

- Irreducible characters form a complete basis for class functions
  - → number of irreps of G = number of conjugacy classes of G

Pf: $f: G \to \mathbb{C}$ is a class function

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

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

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

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

$$\underline{g'' = g'gg'^{-1}}$$

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

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

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

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

$$= f_i\rho_i(g') \quad \Rightarrow \quad [f_i, \rho_i(g)]$$

Schurs Lemma pt. 2 $\Rightarrow$ $\underline{f_i = \lambda_i \mathrm{Id}}$

to find λ_i take the trace

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

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

$$= |G| \langle f, \chi_{\rho_i} \rangle = 0 \text{ by hypothesis}$$

$\Rightarrow f_i = 0$ for every irrep ρ_i

Lets construct a representation called the <u>regular representation</u>

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

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

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

$$[\rho_{reg}(g)]_{e_h e_{g'}} = \vec{e}_h \cdot \rho_{reg}(g)\vec{e}_{g'} = \vec{e}_h \cdot \vec{e}_{gg'} = \begin{cases} 1 & \text{if } h = gg' \\ 0 & \text{otherwise} \end{cases}$$

ρ_{reg} is a sum of irreducible representations

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

$\tilde{F} = \sum_{g \in G} f(g^{-1}) \rho_{reg}(g)$ $\rightarrow$ Schur's lemma tells $\tilde{F} = 0$

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

$\Rightarrow f(g^{-1}) = 0$ for every group element

$\Rightarrow$ $\boxed{\text{Number of irreps = number of conjugacy classes}}$

Turning back to physics: Electrons in solids (ignoring interactions for now)

$$H = \frac{p^2}{2m} + V(\vec{x}) \qquad V(\vec{x}) \text{ - ionic potential}$$

Symmetries of H are a subgroup of $E(3) = \underbrace{\mathbb{R}^3}_{\text{translations}} \rtimes \underbrace{O(3)}_{\text{rotations and reflections}}$

$G \subset \mathbb{E}(3)$ groups G of symmetries of 3D crystals are called space groups

$g \in G$ $\quad V(g^{-1}x) = V(\vec{x})$ $\quad g = \{R \mid \vec{d}\}$

$$g\vec{x} = R\vec{x} + \vec{d}$$

The key thing that defines a crystal: discrete translation symmetry

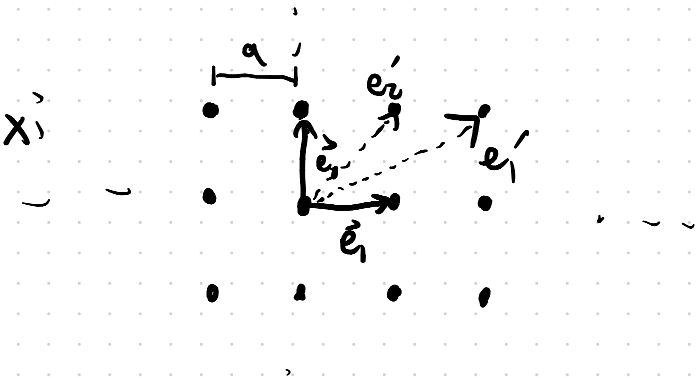
Every space group G has a subgroup

$T = \{\{E \mid n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3\},\ n_i \in \mathbb{Z}\}$ - Bravais lattice

$\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ 3 linearly independent vectors "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:



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

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

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

Primitive unit cell of T: connected subspace of $\mathbb{R}^3$ s.t. no two points can be related by a Bravais lattice translation

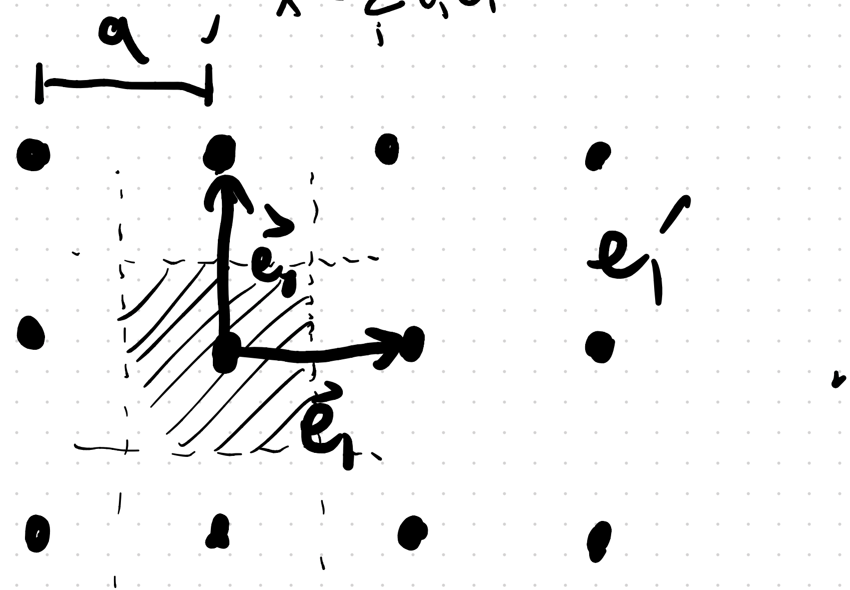
- find primitive lattice vectors $\{\hat{e}_1,\vec{e}_2,\vec{e}_3\}$

$$\left\{ t_1\vec{e}_1 + t_2\vec{e}_2 + t_3\vec{e}_3 \;\middle|\; t_1, t_2, t_3 \in \left[-\tfrac{1}{2}, \tfrac{1}{2}\right) \right\}$$

(t_1, t_2, t_3) reduced coordinates

$$\vec{x} = \sum_i t_i \vec{e}_i$$

Ex:



Alternatively: $\mathbb{R}^3$ is a group, $T \subset \mathbb{R}^3$

$$\mathbb{R}^3 = \bigcup_{(t_1,t_2,t_3)} \left[T + (t_1\vec{e}_1 + t_2\vec{e}_2 + t_3\vec{e}_3) \right]$$

$\Rightarrow$ primitive unit cell is $\mathbb{R}^3 / T$

We know how translations act on quantum states

$\vec{p}$ is a generator of infinitesimal translations

$U_{\vec{t}} = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{t}}$ implements $\vec{t}$ on wavefunctions

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

$\rho: \vec{t} \to U_{\vec{t}}$ is a representation of translations on the Hilbert space of states $|\psi\rangle$

$$\rho(\vec{t}_1)\rho(\vec{t}_2) = U_{\vec{t}_1} U_{\vec{t}_2} = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{t}_1} e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{t}_2} = e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{t}_1+\vec{t}_2)} = \rho(\vec{t}_1+\vec{t}_2)$$

$\rho: T \to \mathcal{U}(\mathcal{H})$ ← group of unitary operators on Hilbert space $\mathcal{H}$

$\vec{t} \to U_{\vec{t}}$

Lets look for invariant subspaces

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

$\downarrow$

$$\lambda_{\vec{t}_1}\lambda_{\vec{t}_2} = \lambda_{\vec{t}_1+\vec{t}_2} \qquad U^{\dagger}_{\vec{t}} = U_{-\vec{t}}$$

$$\lambda_{-\vec{t}} = \lambda^{*}_{\vec{t}}$$

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

crystal momentum

$$\boxed{\text{crystal momentum labels irreducible representations of our Bravais lattice } T}$$

$[H, U_{\vec{t}}] = 0$ since T is a group of symmetries of H

Schur's Lemma: $U_t |\psi_{nk}\rangle = e^{-i\vec{k}\cdot\vec{t}} |\psi_{n\vec{k}}\rangle$ } Bloch's theorem

$$H|\psi_{n\vec{k}}\rangle = E_{n\vec{k}}|\psi_{n\vec{k}}\rangle$$

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

$$\Downarrow$$

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

What are the distinct irreps of T

two irreps $\vec{k}_1$ and $\vec{k}_2$ are the same if

$$e^{-i\vec{k}_1\cdot\vec{t}} = e^{-i\vec{k}_2\cdot\vec{t}} \quad \text{for all } \vec{t}\in T$$

$$e^{i\vec{t}\cdot(\vec{k}_1-\vec{k}_2)} = 1$$

$$(\vec{k}_1-\vec{k}_2)\cdot\vec{t} = 2\pi n_{\vec{t}} \quad \text{for all } \vec{t}\in T$$

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

$$\vec{t} = n_1\vec{e}_1 + n_2\vec{e}_2 + n_3\vec{e}_3$$

primitive reciprocal lattice vectors $\vec{b}_1, \vec{b}_2, \vec{b}_3$

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

$$\vec{k}_1-\vec{k}_2 = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$$

$$\check{T} = \{ m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3 \ , \ m_i \in \mathbb{Z} \}$$ reciprocal lattice

primitive unit cell of $\check{T}$ $= \{ k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3 \mid k_1, k_2, k_3 \in [-\frac{1}{2}, \frac{1}{2}) \}$

index distinct irreps of T

1st Brillouin zone

BZ