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 ρ_1 and 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 $$\frac{1}{|G|}\sum_{g\in G} \chi^*_{\rho_2}(g)\,\chi_{\rho_1}(g) = \begin{cases} 0 & \text{if } \rho_1 \not\cong \rho_2 \\ 1 & \text{if } \rho_1 \cong \rho_2 \end{cases} = \delta_{\rho_1\rho_2}$$

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

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

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

number of conjugacy classes

To see that this is always an equality, we introduce the __regular representation__

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

representation on a vector space of dimension $|G|$

$\mathbb{C}^{|G|}$: Basis vectors $\{\vec{e}_g \mid g \in G\}$

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

$$e_{g_i} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

i

$|G|$

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

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

Let f be a class function $f: G \to \mathbb{C}$

such that $\langle \chi_{\rho_i}, f \rangle = \frac{1}{|G|} \sum_{g \in G} \chi^{*}_{\rho_i}(g) \cdot f(g) = 0$

for every irreducible representation $\rho_i \Rightarrow f = 0$

To show this: For each irrep ρ_i

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

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

Schur's lemma: $f_i = \lambda \, Id$

to find λ

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

$$\sum_{g \in G} f_i(g^{-1}) \chi_{\rho_i}(g) = 0 \text{ by assumption}$$

Now define

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

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

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

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

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

$$f_{reg} = \sum_{g \in G} f(g^{-1}) \underbrace{\rho_{reg}(g)}_{\text{some sum of irreps}} = 0$$

$$\rho_{reg} = \rho_{1} \oplus \rho_{2} \oplus \dots$$

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

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

$\Rightarrow f$ is zero on every group element

$\Rightarrow f = 0$

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

$\rightarrow$ # of irreps of G = # of conjugacy classes of G

$\rightarrow$ conjugacy classes

irreps $\downarrow$

	C_1	C_2	C_3
ρ_1			
ρ_2		Squere	
ρ_3			

Decomposition of representations:

let $\rho : G \to U(V)$ be a representation of a group

let $\{\rho_i\}$ be the irreps for the group

define $P_i = \frac{\dim \rho_i}{|G|} \sum_{g \in G} \chi^*_{\rho_i}(g)\, \rho(g)$

since ρ is reducible: $\rho(g) = U \begin{pmatrix} \rho_1(g) & & \\ & \rho_2(g) & \\ & & \ddots \end{pmatrix} U^\dagger$

$$= U \bigoplus_j \rho_j(g) U^\dagger$$

$$P_i = \frac{\dim \rho_i}{|G|} U \left[\sum_{g \in G} \chi^*_{\rho_i}(g) \bigoplus_j \rho_j(g) \right] U^\dagger$$

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

$$\Big\downarrow \mu = i$$

$$\sum_{g \in G} \chi^*_{\rho_2}(g) [\rho_1(g)]^{j\nu} = \begin{cases} 0 & \text{if } \rho_1 \neq \rho_2 \\ \frac{|G|}{\dim \rho_1} \delta_{j\nu} & \text{if } \rho_1 = \rho_2 \end{cases}$$

$$P_i = \frac{\dim \rho_i}{|G|} U \underbrace{\bigoplus_j \left(\frac{|G|}{\dim \rho_i} \delta_{\rho_i \rho_j} \right)} U^\dagger$$

$P_i = 0$ on all vectors that do not transform in the irrep ρ_i

$= \mathbb{1}$ (up to a unitary transformation) on vectors that do transform in ρ_i

$\Rightarrow$ P_i projects onto the subspaces that transform in ρ_i

if $\{|w_a^i\rangle\}$ that span the invariant subspace for ρ_i $P_i = \sum_a |w_a^i\rangle\langle w_a^i|$

$$P_i\, \rho(g)\, P_i$$

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

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

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

Rigid symmetries of H

$$G < E(3) = \underset{\text{translations}}{\mathbb{R}^3} \rtimes \underset{\text{rotations \& reflections}}{O(3)}$$

$$G = \{ g \in E(3) \mid V(\vec{x}) = V(g^{-1}\vec{x}) \} \qquad g = \{ \underset{O(3)}{R} \mid \underset{\mathbb{R}^3}{\vec{d}} \} \qquad g\vec{x} = [R]\vec{x} + \vec{d}$$

$\downarrow$

These groups of rigid symmetries of crystals are space groups

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

Every space group must contain a Bravais lattice subgroup $T = \left\{ \{E \mid \sum_i n_i \vec{e}_i\} \mid n_i \in \mathbb{Z} \right\}$

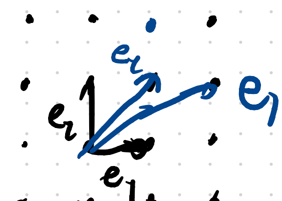
$\vec{e}_1, \vec{e}_2, \vec{e}_3$ linearly independent
"primitive lattice vectors"

$T \triangleleft G$ is a normal subgroup

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

Ex: 2D Bravais lattice

$\vec{e}_1 = (a, 0)$
$\vec{e}_2 = (0, a)$



$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \vec{e}_1 \\ \vec{e}_2 \end{pmatrix}$$

$$\begin{pmatrix}\vec{e}_1\\ \vec{e}_2\end{pmatrix} = \begin{pmatrix}2 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}\vec{\bar{e}}_1\\ \vec{\bar{e}}_2\end{pmatrix}$$

$\begin{pmatrix}a & b\\ c & d\end{pmatrix}^{-1}$ is also integer valued

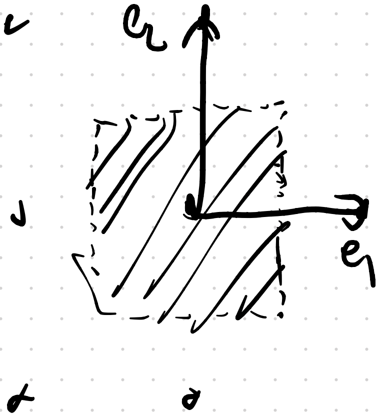
$$\begin{pmatrix}\vec{\bar{e}}_1\\ \vec{\bar{e}}_2\end{pmatrix} = \begin{pmatrix}1 & -1\\ -1 & 2\end{pmatrix}\begin{pmatrix}\vec{e}_1\\ \vec{e}_2\end{pmatrix}$$

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

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

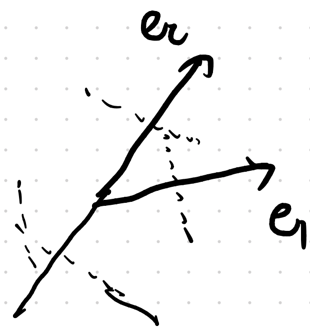
$$= \left\{ \left\{ E \,\middle|\, \sum_i n_i \vec{e}_i + \vec{v} \right\} \,\middle|\, \vec{v} \in \mathbb{R}^3,\ n_i \in \mathbb{Z} \right\}$$

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

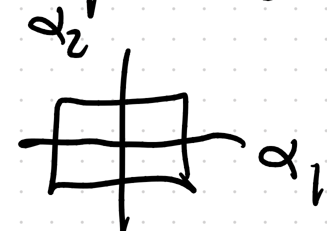


Wigner-Seitz construction

$(\alpha_1, \alpha_2, \alpha_3)$ - reduced coordinates for points in the unit cell



$\alpha_1 \vec{e}_1 + \alpha_2 \vec{e}_2$



Lets look @ how T is represented on wavefunctions

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

Momentum operator

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

$$\vec{t} \to U_t = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{t}}$$

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

$$U_{t_1} U_{t_2} = U_{t_2} U_{t_1} = U_{t_1+t_2}$$ ← Abelian: All irreps are 1D

We can simultaneously diagonalize all $U_{\vec{t}}$

$$U_{\vec{t}} = \begin{pmatrix} \lambda_1(t_1) & & & \\ & \lambda_2(t) & & \\ & & \lambda_3(t) & \\ & & & \ddots \end{pmatrix}$$

what are the 1D irreps of T

$$\lambda(0) = 1$$

$$\lambda(t)^* = \lambda(-t)$$

$$\lambda(t_1)\lambda(t_2) = \lambda(t_1 + t_2)$$

$$\lambda(t) = e^{-i\vec{k}\cdot\vec{t}}$$

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

What are the distinct maps

$\lambda_{k_1}, \lambda_{k_2}$ are the same if $\lambda_{k_1}(t) = \lambda_{k_2}(t)$ forall $\vec{t} \in T$

$$e^{-i\vec{k}_1 \vec{t}} = e^{-i k_2 \cdot \vec{t}} \qquad e^{i(k_1 - k_2)\cdot \vec{t}} = 1 \text{ for all } t \in T$$

$$\boxed{(k_1 - k_2)\cdot \vec{t} = 2\pi n_{\vec{t}}} \qquad \vec{t} = n_1 \vec{e}_1 + n_2 \vec{e}_2 + n_3 \vec{e}_3$$

Given $\{\vec{e}_1\}$ lets introduce

primitive reciprocal lattice vectors $\{\vec{b}_1, \vec{b}_2, \vec{b}_3\}$ $\qquad \vec{b}_i \cdot \vec{e}_j = 2\pi\delta_{ij}$

$$k_1 - k_2 = \sum_i m_i \vec{b}_i \Rightarrow \lambda_{k_1} = \lambda_{k_2}$$

reciprocal lattice $\check{T} = \{\sum_i m_i \vec{b}_i \mid m_i \in \mathbb{Z}\}$

Space of distinct irreps of T - unit cell in $\check{T}$ - 1st Brillouin zone $= \{\sum_i k_i \vec{b}_i \mid k_i \in (-\frac{1}{2}, \frac{1}{2})\}$

$\vec{k}$ - crystal momentum $\qquad \vec{e} = a\vec{x}$

$\vec{b} = \frac{2\pi}{a}$

$$\left\{ k \frac{2\pi}{a}\hat{x},\ k \in \left[-\frac{1}{2}, \frac{1}{2}\right] \right\}$$