Lecture 7

Reminders:
- Class on 9/19 and 9/21 will run an extra 40mins
- HW 2 will be posted 9/19, due 10/3

Last lecture: Space group $G \subset E(3)$ that can be symmetry groups of 3D crystals

Every space group has a Bravais lattice $T \subset G$

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

2D example: square lattice $\vec{e}_1 = (a,0)$
$\vec{e}_2 = (0,a)$

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

Primitive unit cell of T: connected subset of space s.t. no two points can be related by a Bravais lattice translation

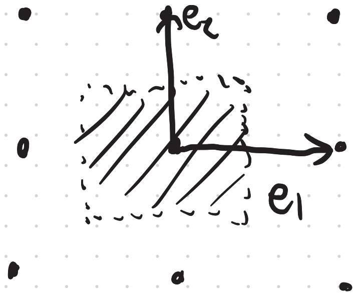
given $\vec{e}_1, \vec{e}_2, \vec{e}_3$ one choice of (primitive) unit cell

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

can express points in the unit cell in reduced coordinates

$\vec{x} = (t_1, t_2, t_3) \rightsquigarrow \vec{x} = \sum_i t_i \vec{e}_i$

Ex



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

T is a symmetry group of H, $V(\vec{x}) = V(\vec{x} - \vec{t})$ for all $\vec{t} \in T$

We know how translations act on wavefunctions

$$U_{\vec{t}} = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{t}}$$ generates the translation $\vec{t}$

on Q.M. states

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

$\{ U_{\vec{t}} \,|\, \vec{t} \in T \}$ is a representation of $\vec{t}$

$$(*) \quad U_{\vec{t}_1} U_{\vec{t}_2} = e^{-i\vec{p}\cdot\vec{t}_1/\hbar} e^{-i\vec{p}\cdot\vec{t}_2/\hbar} = e^{-i\frac{\vec{p}}{\hbar}(t_1+t_2)} = U_{\vec{t}_1+\vec{t}_2}$$

Lets look for invariant subspaces

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

$$U_{\vec{t}}|\psi\rangle = \lambda_{\vec{t}}|\psi\rangle$$

$\lambda_{t_1}\lambda_{t_2} = \lambda_{t_1+t_2}$ from (*)

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

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

irreducible representations of T are labelled by $\vec{k}$ - crystal momentum

Aside: Say we have a group G that is abelian: $g_1 g_2 = g_2 g_1$

$\to$ all irreducible reps of G are 1-dimensional

Suppose ρ is a rep of G

G abelian $\Rightarrow$ $\rho(g_1)\rho(g_2) = \rho(g_2)\rho(g_1)$

$\to$ $[\rho(g_1), \rho(g_2)] = 0$

So we can simultaneously diagonalise all $\rho(g)$ $\to$ each eigenvector spans a 1D invariant subspace

Schur's lemma $\Rightarrow$ Eigenstates of H can be labelled by irreps of T,

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

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

- Bloch's theorem

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

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

What are the distinct irreps?

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

for all $\vec{t}$ in T

$$\Rightarrow (\vec{k}_1 - \vec{k}_2) \cdot \vec{t} = 2\pi n$$

to index irreps, we can introduce the reciprocal lattice

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

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

column vectors

$$(\vec{b}_1, \vec{b}_2, \vec{b}_3) = 2\pi \begin{pmatrix} \vec{e}_1^T \\ e_2^T \\ e_3^T \end{pmatrix}^{-1}$$

$$\check{T} = \{ n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3 \mid n_1, n_2, n_3 \in \mathbb{Z} \}$$ reciprocal lattice

k_1, k_2 index the same irrep of T if $k_1 - k_2 \in \check{T}$

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

1st Brillouin zone

$$\left(\text{w/ periodic B/Cs} \quad (U_{\vec{t}})^N |\psi\rangle = |\psi\rangle \right)$$

$$\left(\qquad k = \frac{2\pi}{N} n \vec{b} \qquad \right)$$

What about other rigid transformations:

1. What transformations can appear in a space group?

2. What affect do they have?

To address this, we should note $T \triangleleft G$ is a normal subgroup of the space group

lets take $g = \{R | \vec{d}\} \notin T$ $\quad \{E | \vec{t}\} \in T$

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

$$\boxed{\begin{aligned}&\{R_1|\vec{d}_1\}\{R_2|\vec{d}_2\}\\&=\{R_1R_2|\vec{d}_1+R_1\vec{d}_2\}\end{aligned}}$$

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

$$= \{E|R^{-1}\vec{t}\} \in T$$ if T consists of all translation symmetries

for any space group, we can look @ the quotient

$\overline{G} = G/T$ - point group of G

1st isomorphism theorem: if I find φ a homomorphism s.t. $\ker\varphi = T$

then $\mathrm{Im}\,\varphi \cong G/T \cong \overline{G}$

$\varphi : G \to O(3)$

$\varphi(\{R|\vec{d}\}) = R \qquad \ker \varphi = \{\{E|\vec{t}\}\} = T$

$\to$ Point group $\overline{G}$ is a subgroup of $O(3)$

Important result - <u>Crystallographic Restriction Theorem</u>

given a Bravais lattice T and a rotation R

if R is a symmetry of T $(R\vec{t} \in T) \to R$ is

a rotation by either $0°$ $60°$, $90°$, $120°$, $180°$

$0 \quad \frac{\pi}{3} \quad \frac{\pi}{2} \quad \frac{2\pi}{3} \quad \pi$

Pf: lets pick primitive lattice vectors $\vec{e}_1, \vec{e}_2, \vec{e}_3$

Construct a matrix $R_{ij} = \vec{e}_i^{\,T} \cdot R\vec{e}_j$

R is a symmetry of T, $Re_j \in T$

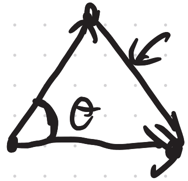
$\Rightarrow R_{ij}$ has to be an integer matrix

$\Rightarrow \sum_i R_{ii} = \operatorname{tr} R \in \mathbb{Z}$

but $\operatorname{tr} R$ is basis invariant so lets evaluate it in a basis aligned with the axis of rotation

$$R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}$$

θ is angle of rotation



$$\operatorname{tr} R = 1 + 2\cos\theta \in \mathbb{Z}$$

$$1 + 2\cos\theta = 0, \pm 1, \pm 2, \pm 3, \ldots$$

$$\Rightarrow \cos\theta = 0, \pm\frac{1}{2}, \pm 1$$

$$\boxed{\theta = \pm\frac{\pi}{2}, \frac{\pi}{3}, \frac{2\pi}{3}, 0, \pi}$$

There are only 32 subgroups of $O(3)$ consistent w/ this theorem [10 are pt groups of 2D crystals]

Group	Hermann-Maugin Notation	Schöflies Notation
• trivial group	1	C_1
• $\langle C_{2z} \rangle$	2	C_2
• $\langle C_{3z} \rangle$	3	C_3
• $\langle C_{4z} \rangle$	4	C_4
• $\langle C_{6z} \rangle$	6	C_6

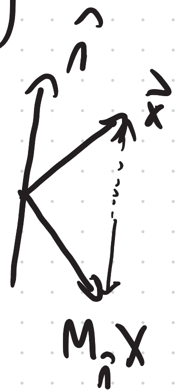
$\langle g_1, g_2, \ldots \rangle$ the group generated by $g_1, g_2, \ldots$

$C_{n\hat{r}}$ - $\frac{2\pi}{n}$ rotation about $\hat{r}$

We can also have reflection symmetries

(mirror)

$M_{\hat{n}}$



Ex $M_x : (x, y, z) \to (-x, y, z)$

$\langle M_x \rangle$	m	C_s
$\langle C_{2z}, M_x \rangle$	$mm2$	C_{2v}
$\langle C_{3z}, M_x \rangle$	$3m$	C_{3v}
$\langle C_{4z}, M_x \rangle$	$4mm$	C_{4v}

$\langle C_{6z}, M_x \rangle$	$6mm$	C_{6v}

Inversion symmetry $I: (x,y,z) \to (-x,-y,-z)$

https://cryst.ehu.es

$C_{2z}: (x,y,z) \to (-x,-y,z)$

$I: (x,y,z) \to (-x,-y,-z)$

$IC_{2z} = M_z: (x,y,z) \to (x,y,-z)$

$$\vec{e}_1 = \begin{pmatrix} e_1^a \\ e_1^b \\ e_1^c \end{pmatrix} \qquad \vec{e}_2 = \begin{pmatrix} e_2^a \\ e_2^b \\ e_2^c \end{pmatrix} \qquad \vec{e}_3 = \begin{pmatrix} e_3^a \\ e_3^b \\ e_3^c \end{pmatrix}$$

$$\left[\begin{pmatrix} e_1^a & e_2^a & e_3^a \\ e_1^b & e_2^b & e_3^b \\ e_1^c & e_2^c & e_3^c \end{pmatrix}^T \right]^{-1}$$

$$b_1 = 2\pi \frac{e_2 \times e_3}{e_1 \cdot (e_2 \times e_3)} \qquad b_2 = 2\pi \frac{e_1 \times e_3}{e_1 \cdot (e_2 \times e_3)}$$

$$b_3 = 2\pi \frac{e_1 \times e_2}{e_1 \cdot (e_2 \times e_3)}$$

1D irreps of T

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