Lect 12: Representations of space group

1. Representations of translation group

Translational group is an Abelian group, hence, all its representations will be one-dimensional.

$$\vec{l} = \vec{a}_1 l_1 + \vec{a}_2 l_2 + \vec{a}_3 l_3 \iff \vec{K} = \vec{b}_1 K_1 + \vec{b}_2 K_2 + \vec{b}_3 K_3$$

reciprocal lattice vector

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

$$\Rightarrow \vec{l} \cdot \vec{K} = 2\pi \sum_{i=1}^{3} l_i K_i \text{ , where } l_i, K_i \text{ are integers.}$$

if R is a point group symmetry, of the lattice vector $\vec{l}$,

then $(R\vec{K}) \cdot \vec{l} = \vec{K} \cdot R^{-1}\vec{l} = \vec{K} \cdot \vec{l}' = \text{integer} \cdot 2\pi$

$\Rightarrow$ R is also a point-group symmetry of the reciprocal lattice.

It's representation can be denoted by the Bloch wave vector

$$\boxed{\vec{k} = \sum_{j=1}^{3} \vec{b}_j k_j , \quad k_j = P_j / N_j ,}$$

where N_j is the number of sites along the $\vec{a}_j$ direction.

Since $T = T^{(1)} \otimes T^{(2)} \otimes T^{(3)}$, where $T^{(1,2,3)}$ are the cyclic groups reprensenting translations along $\vec{a}_{1,2,3}$ respectively. $k_{j=1,2,3} = P_j/N_j$ with P_j represents the ~~representation~~ index of the cyclic group hence $$\boxed{\begin{aligned} &D^{\vec{k}}(\vec{l}) = \exp\left[-i2\pi \sum_{j=1}^{3} k_j l_j\right], \quad 0 \le k_j < 1 \\ &\vec{k} = \sum k_j \vec{b}_j, \quad k_j = \quad p_j/N_j \end{aligned}}$$

$$\boxed{\begin{aligned} &T(\vec{l})\psi_{\vec{k}}(\vec{r}) \\ &= e^{-i\vec{k}\cdot\vec{l}}\psi_{\vec{k}}(\vec{r}) \end{aligned}}$$

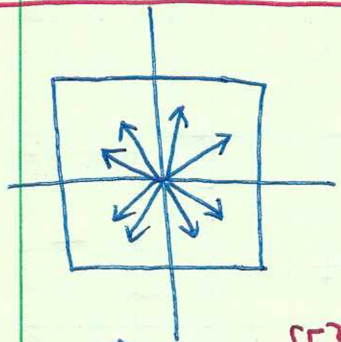
$\vec{k}$: wavevector (Bloch), difference $\vec{K}$ and $\vec{k}'$ with $\vec{k}' = \vec{k} + \vec{K}$ are equivalent correponding to the same representation.

Brillionin Zone: unite cells in recepirocal space — c.f. Solid state physics

2 (*) $\overbrace{\text{wave vector group}}^{\text{Subgroup}}$ and star of $\vec{k}$

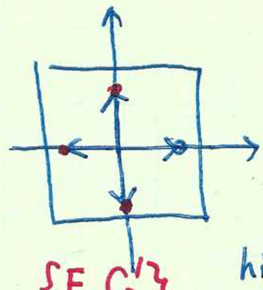
G_k

The group of wavevector $G_{\vec{k}}$ is formed by the set of space group operations leaving $\vec{k}$ invariant, or into $\vec{k}' = \vec{k} + \vec{K}_m$. ($\vec{K}_m$ is a vector of the reciprocal lattice. The set of $\{\vec{k}''\}$ obtained by carrying out all point group operations on $\vec{k}$ is called $\boxed{\text{the star of } \vec{k}.}$ ← coset



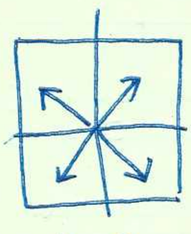
$\{E\}$

8 $\vec{k}$ in Star



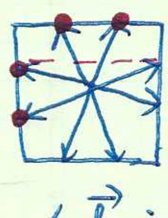
$\{E, C_2'\}$

high symmetry lines



$\{E, C_2''\}$

4 $\vec{k}$ is Star

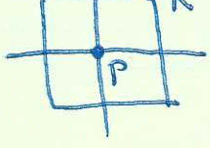


4 $\vec{k}$ in Star

$\{E, C_2'\}$

2 $\vec{k}$ in Star

$\{E, C_2\ 2C_2'\}$



1 $\vec{k}$ in Star

$\{E, C_2\ 2C_4, 2C_2', 2C_2''\}$

③

Consider a m-dimensional unitary representation of space group.

In a proper basis, it's form for the subgroup $T(\vec{l})$ taking the following diagonal form

$$\boxed{D(E,\vec{l}) = \text{diag}\{ e^{-i\vec{k}_1\cdot\vec{l}},\ e^{-i\vec{k}_2\cdot\vec{l}},\ \ldots\ e^{-i\vec{k}_m\cdot\vec{l}} \}.}$$

Since $g^{-1}(R,\vec{\alpha})\, g(E,\vec{l})\, g(R,\vec{\alpha}) = g(E, R^{-1}\vec{l})$

$$D(E, R^{-1}\vec{l}) = \text{diag}\{ e^{-i\vec{k}_j\cdot R^{-1}\vec{l}} \} = \text{diag}\{ e^{-i R\vec{k}_j\cdot\vec{l}} \}$$

which is similiar to $D(E,\vec{l}) = \text{diag}\{ e^{-i\vec{k}_j\cdot\vec{l}} \}$, hence $R\vec{k}_j$ must equal a $\vec{k}_i$ or its equavilent $\vec{k}_i + \vec{K}$.

Based on $D^{-1}(R,\vec{\alpha})\, D(E,\vec{l})\, D(R,\vec{\alpha}) = D(E, R^{-1}\vec{l})$

$$\Rightarrow D_{\tau\tau}(E,\vec{l})\, D_{\tau p}(R,\vec{\alpha}) = D_{\tau p}(R,\vec{\alpha})\, D_{pp}(E, R^{-1}\vec{l})$$

$$e^{-i\vec{k}_\tau\cdot\vec{l}}\, D_{\tau p}(R,\vec{\alpha}) = D_{\tau p}(R,\vec{\alpha})\, e^{-i R\vec{k}_p\cdot\vec{l}}$$

$$\Rightarrow \boxed{\text{if } D_{\tau p}(R,\vec{\alpha}) \neq 0 \Rightarrow R\vec{k}_p = \vec{k}_\tau + \vec{K}}$$

Since $D(R,\vec{\alpha})$ is irreducible, the set of $\{\vec{k}_i\}$ must form a star of $\vec{k}$. Otherwise, if it contains two stars, $\{\vec{k}\}$ and $\{\vec{k}'\}$, they cannot be connected by R operations, then $D(R,\vec{\alpha})$ is reducible.

Let's rewrite the $D(E,\vec{l})$ by putting equivalent $\vec{k}$'s together

$$\boxed{D(E,\vec{l}) = \text{diag}\{ \underbrace{e^{-i\vec{k}_1\cdot\vec{l}} \ldots e^{-i\vec{k}_1\cdot\vec{l}}}_{d},\ \underbrace{e^{-i\vec{k}_2\cdot\vec{l}} \ldots e^{-i\vec{k}_2\cdot\vec{l}}}_{d},\ \ldots\ \underbrace{e^{-i\vec{k}_q\cdot\vec{l}} \ldots e^{-i\vec{k}_q\cdot\vec{l}}}_{d} \}}$$

$\{\vec{k}_1, \cdots \vec{k}_q\}$ are a star, and "q" is the branch number of this star. Since $\{R\vec{k}_i\}$ is just the set of $\{\vec{k}_i\}$, ~~and~~ the permutation must take ~~the equivalent unit for~~ between the subsets of equivalent $\{\underbrace{k_i, k_i \cdots k_i}_{d}\}$ and ~~$\{\alpha\}$~~ $\{\underbrace{k_j \cdots k_j}_{d}\}$, hence their degenercies must be equal. We have

> Every irreducible representation of a space group corresponds to a specific star of wavevector. The dimension of representation and the branching # of the star satisfy $m = qd$.

3. Representation matrix of space group

: $m = qd$. We devide the $m \times m$ dimensional matrix $D(R, \vec{\alpha})$ for the space group element $g(R, \vec{\alpha})$ into q^2 $d \times d$ blocks of $D_{\mu\nu}$, i.e

$$D(R, \vec{\alpha}) = \begin{pmatrix} D_{11}(R, \vec{\alpha}) & \cdots & D_{1q}(R, \vec{\alpha}) \\ \vdots & & \\ D_{q1}(R, \vec{\alpha}) & \cdots & D_{qq}(R, \vec{\alpha}) \end{pmatrix}$$ where $D_{\mu\nu}(R, \vec{\alpha})$ is a $d \times d$ matrix.

Below we will prove that for each row and column, there only exist only one small matrix nonzero. And such a nonzero matrix is determined by the group of wavevecter $G_{\vec{k}}$.

☆ For translation $T(\vec{l})$. Since k_μ and k_ν are two non-equivalent elements in the star, and all $\vec{k}$'s in the same small matrix are equivalent, we have

$$\boxed{D_{\mu\nu}(E,\vec{l}) = I_{d\times d}\, \delta_{\mu\nu}\, e^{-i\vec{k}_\mu\cdot\vec{l}}}$$

☆ Consider $g(R,\vec{\alpha})$,

Let's pick up one wavevector in the star, say, $\vec{k}_1$, and its group of wavevector $G_{\vec{k}_1}$ is denoted by $\{P\}$. i.e. $P\vec{k}_1 \equiv \vec{k}_1 \mod(\vec{b}_i)$

The the coset $R_\mu\{P\} \rightarrow R_\mu\vec{k}_1 \equiv \vec{k}_\mu \mod(\vec{b}_i)$,

and $\mu = 1, 2, \cdots q$.

According to $D(E,\vec{l})\,D(R,\vec{\alpha}) = D(R,\vec{\alpha})\,D(E,R^{-1}\vec{l})$

$$D_{\lambda\delta}(E,\vec{l})\,D_{\delta\gamma}(R,\vec{\alpha}) = D_{\lambda\delta}(R,\vec{\alpha})\,D_{\delta\gamma}(E,R^{-1}\vec{l})$$

(The greek indices refer to the Block index). $\Rightarrow$

$$\delta_{\lambda\delta}\, e^{-i\vec{k}_\lambda\cdot\vec{l}}\, D_{\delta\gamma}(R,\vec{\alpha}) = D_{\lambda\delta}(R,\vec{\alpha})\,\delta_{\delta\gamma}\, e^{-i\vec{k}_\gamma\cdot R^{-1}\vec{l}}$$

$$e^{-i\vec{k}_\lambda\cdot\vec{l}}\, D_{\lambda\gamma}(R,\vec{\alpha}) = D_{\lambda\gamma}(R,\vec{\alpha})\, e^{-iR\vec{k}_\gamma\cdot\vec{l}}$$

$$\boxed{\text{Hence } D_{\lambda\gamma}(R,\vec{\alpha}) \neq 0, \text{ iff } R\vec{k}_\gamma = \vec{k}_\lambda}$$

For a given R, and λ, there only exists a single γ $\vec{k}_\gamma = R^{-1}\vec{k}_\lambda$

a given R and γ, there is only a single $\vec{k}_\lambda = R\vec{k}_\gamma$. nonzero

Hence, for each row and column, there is only one small matrix

☆ For a general $g(R,\vec{\alpha})$, consider it's representation matrix

$D_{\rho\mu}(R,\vec{\alpha})$ with μ-fixed, and ρ runs from 1 to q.

consider $R\vec{k}_\mu = R R_\mu \vec{k}_1$ ~~$= R_\nu P$~~, check $R R_\mu$ belonging to

the coset of $R_\nu\{P\}$, then $\boxed{R R_\mu = R_\nu P} \Rightarrow \boxed{R\vec{k}_\mu = \vec{k}_\nu}$

$$\Rightarrow \quad R = R_\nu P R_\mu^{-1} \quad \Rightarrow g(R,\vec{\alpha}) = g(R_\nu \vec{t}_\nu)\, g(P, t_p)\, g^{-1}(R_\mu, t_\mu)$$

For a given space group, and $\vec{k}_1$, once R and R_μ are fixed.

t_μ $\vec{\alpha}$, (R_ν, t_ν), (P, t_p) are also determined.

Then $D_{\rho\mu}(R,\vec{\alpha})$ is nonzero, if and only if $\rho = \nu$ for $R\vec{k}_\mu = \vec{k}_\nu$

and $$D_{\nu\mu}(R,\vec{\alpha}) = \sum_{\tau,\lambda} D_{\nu\tau}(R_\nu, \vec{t}_\nu)\, D_{\tau\lambda}(P, t_p)\, D^*_{\mu\lambda}(R_\mu, \vec{t}_\mu)$$

$$\begin{cases} D_{\nu\tau}(R_\nu, \vec{t}_\nu) \neq 0 \ (\nu \text{ given}) \text{ iff } \quad R_\nu \vec{k}_\tau = \vec{k}_\nu \Rightarrow \vec{k}_\tau = R_\nu^{-1} k_\nu = \vec{k}_1 \\ \text{i.e. } \tau = 1 \\ D_{\mu\lambda}(R_\mu, \vec{t}_\mu) \neq 0 \ (\mu \text{ given}) \text{ iff } \ \lambda = 1 \end{cases}$$

$$\Rightarrow \boxed{D_{\nu\mu}(R,\vec{\alpha}) = D_{\nu 1}(R_\nu \vec{t}_\nu)\, D_{11}(P, t_p)\, D^*_{\mu 1}(R_\mu, t_\mu)}$$

Actually we can set $D_{\mu 1}(R_\mu, t_\mu) = I_{d\times d}$,

This corresponds to a phase convention between the set of state of $\vec{k}_1$ to that set of states of $\vec{k}_\mu$

i.e we defin $|\psi_i(\vec{k}_\mu)\rangle = g(R_\mu, t_\mu)\,|\psi_i(\vec{k}_1)\rangle$

for $i = 1, 2, \cdots d$

$$\Rightarrow D_{\mu 1, ij}(R_\mu, t_\mu) = \langle \psi_i(\vec{k}_\mu)|\, g(R_\mu, t_\mu)\, |\psi_j(\vec{k}_1)\rangle$$

$$= \langle \psi_i(\vec{k}_1)|\, g^{-1}(R_\mu, t_\mu)\, g(R_\mu, t_\mu)\, |\psi_j(\vec{k}_1)\rangle = \delta_{ij}$$

With this convention $\Rightarrow$

$$\boxed{D_{\nu\mu}(R, \vec{\alpha}) = D_{11}(P, t_p)} \quad \text{or} \quad D_{\rho\mu}(R, \vec{\alpha}) = \delta_{\rho\nu}\, D_{11}(P, t_p)$$

where $\vec{k}_\nu = R\vec{k}_\mu$

Hence, Reps of space groups are completely determined by the irreducible Reps of the group of wavevector $G(\vec{k})$. where $\vec{k}$ is any one in the star. $D_{11}(P, t_p)$ is a d-dimensional $d\times d$ irreducible Rep for the group of wavevector.

⊛ Multiplier algebra

Consider group operations $g(R_1, \vec{\alpha}_1)$ and $g(R_2, \vec{\alpha}_2)$ in the group of the wave vector $\vec{k}$. Then $\boxed{g(R_1 \vec{\alpha}_1)\, g(R_2, \vec{\alpha}_2) = g(E, \vec{t})\, g(R_1 R_2, \vec{\alpha})}$ where $\vec{\alpha}$ is fractional translation associated with $R_1 R_2$, and $\boxed{\vec{t} = \vec{\alpha}_1 + R_1 \vec{\alpha}_2 - \vec{\alpha}}$.

Consider a Bloch wave state $\psi_{\vec{k}}(\vec{r})$

$$\boxed{g(R_1, \vec{\alpha}_1)\, g(R_2, \vec{\alpha}_2)\, \psi_{\vec{k}}(\vec{r}) = e^{-i\vec{k}\cdot\vec{t}}\, g(R_1 R_2, \vec{\alpha})\, \psi_{\vec{k}}(\vec{r})}$$

Due to the phase of $e^{-i\vec{k}\cdot\vec{t}}$, actually the ~~plane~~ Bloch wave state form a projective representation, or the multiplier representation.

— Lyubarskii (1960). Döring (1959).

We define the following operation when operating on $\psi_{\vec{k}}(\vec{r})$

$$O(R_1) \equiv g(R_1, \vec{\alpha}_1)\, e^{i\vec{k}\cdot\vec{\alpha}_1} = g(R_1, \vec{\alpha}_1 + \vec{l})\, e^{i\vec{k}\cdot(\vec{\alpha}_1 + \vec{l})}$$

hence $O(R_1)$ represents all the $g(R_1, \vec{\alpha}_1 + \vec{l})$

Then $\boxed{O(R_1)\, O(R_2) = \lambda(R_1, R_2)\, O(R_1 R_2)}$ ← where $\lambda(R_1, R_2) = e^{i\vec{k}\cdot(\vec{\alpha}_2 - R_1\vec{\alpha}_2)}$

$$\vec{k}\cdot R_1\vec{\alpha}_2 = R_1^{-1}\vec{k}\cdot\vec{\alpha}_2 = (\vec{k} - \vec{K}_1)\cdot\vec{\alpha}_2 \quad \leftarrow \text{since } g(R_1 \vec{\alpha}_1) \in G_{\vec{k}}$$

$\Rightarrow \lambda(R_1, R_2) = e^{i\vec{K}_1\cdot\vec{\alpha}_2}$, where $\vec{K}_1$ is some reciprocal lattice vector (could be zero, or nonzero)

⊛ Representations for the symmorphic space groups.

It's possible to set all fractional translations to 0, i.e. $\vec{\alpha}=0$ by a suitable choice of origin. Hence $\lambda(R_1, R_2)=1$. Then for the group of wavevector $\vec{k}$,

$$\boxed{\begin{aligned} D_{11}^{\vec{k},j}(R,\vec{l}) &= e^{-i\vec{k}\cdot\vec{l}} D^j(R) \\ \text{and} \quad \chi_{11}^{\vec{k},j}(R,\vec{l}) &= e^{-i\vec{k}\cdot\vec{l}} \chi^j(R) \end{aligned}}$$

← where $\vec{l}$ is integer

⊛ non-symmorphic space groups

① Interior points of the Brillouin zone. In this case, both $\vec{k}$ and $R_1^{-1}\vec{k}$ are inside BZ, hence, their difference must be zero and ~~λ~~ $\lambda(R_1, R_2)=0$. In this case

$$D_{11}^{\vec{k},j}(R,\vec{t}_R) = e^{-i\vec{k}\cdot\vec{t}_R} D^j(R), \quad \text{where } \underset{g(R,\vec{t}_R)}{g} \in G_{\vec{k}}.$$

② Zone boundary points containing a one dimension representation of the $O(R_1)O(R_2) = \lambda(R_1,R_2)\,O(R_1R_2)$.

If there exists a representation $\nu(R)$ satisfying

$$\nu(R_1)\,\nu(R_2) = \lambda(R_1,R_2)\,\nu(R_1R_2), \text{ then}$$

$$\boxed{\frac{O(R_1)}{\nu(R_1)}\cdot\frac{O(R_2)}{\nu(R_2)} = \frac{O(R_1R_2)}{\nu(R_1R_2)}}$$

← then $\dfrac{O(R)}{\nu(R)}$ follow the point group multiplication then $\boxed{D_{11}^{\vec{k},j}(R,\vec{t}_R) = e^{-i\vec{k}\cdot\vec{t}_R}\, \nu(R_1)\, D^j(R)}$

Representations of a multiplier group that differ by a factor transformation $D'(R) = \nu(R)\, D(R)$ are called p-equivalent.

③ if $R_1 R_2 = R_2 R_1$, but $\lambda(R_1,R_2) \neq \lambda(R_2,R_1)$

then
$$\left.\begin{aligned} O(R_1)O(R_2) &= \lambda(R_1R_2)\, O(R_1R_2) \\ O(R_2)O(R_1) &= \lambda(R_2,R_1)\, O(R_2R_1) \end{aligned}\right\} \Rightarrow \boxed{O(R_1)O(R_2) = \frac{\lambda(R_1,R_2)}{\lambda(R_2R_1)}\, O(R_2)O(R_1)}$$

there must appear degenercies — 1D representations impossible.