Lecture 13

M_y $(n\,l\,m)$

$\hookrightarrow M_{010}$ relative to the cartesian basis vectors

Ex: point group $2^d = \langle C_{2z} \rangle$

$C_{2z}^2 = \bar{E}$

single-valued

double valued

	E	$\bar{E}$	C_{2z}	C_{2z}^{-1}
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
$\bar{\Gamma}_3$	1	-1	$-i$	$+i$

$\Gamma_4 \mid 1 \quad -1 \quad +i \quad -i$

Question: Can we add a representation matrix for time-reversal to each of these irreps

Γ_1: $\Gamma_1(T) = U_T \mathcal{K}$

$\Gamma_1(T)^2 = +1$

$\rightarrow \Gamma_1(T) = \mathcal{K}$

Γ_2: $\Gamma_2(T) = \mathcal{K}$

A <u>corepresentation</u> is a representation with both unitary and antiunitary matrices

$\bar{\Gamma}_3$: $\bar{\Gamma}_3(T)^2 = -1$

$$\bar{\Gamma}_3^{-1}(T)\,\bar{\Gamma}_3(g)\,\bar{\Gamma}_3(T) = \bar{\Gamma}_3(g)$$

$$\bar{\Gamma}_3(T) = \alpha K \qquad \bar{\Gamma}_3(T)^2 = \alpha\alpha^* = -1$$

This is impossible

$\bar{\Gamma}_3$ and $\bar{\Gamma}_4$ are not corepresentations

$\bar{\Gamma}_3 \oplus \bar{\Gamma}_4 = \rho$

$$\rho(C_{2z}) = \begin{pmatrix} -i & \\ & i \end{pmatrix} = -i\sigma_z$$

$$\rho(T) = i\sigma_y K$$

ρ is an $\underbrace{\text{irreducible corepresentation}}$ of 2^d with TRS

$\rightarrow \bar{\Gamma}_3\bar{\Gamma}_4$

Herman Maugin - Time-reversal is denoted $1'$

"physically irreducible representations" on BCS

c.f. Bradley and Cracknell §4.6
Ch 7

How does T act on $\vec{k}$

$$T|\psi_{n\vec{k}}\rangle = |\varphi\rangle$$

$$U_{\vec{t}}|\varphi\rangle = U_{\vec{t}}\,T|\psi_{n\vec{k}}\rangle$$

$$= T\,U_{\vec{t}}|\psi_{n\vec{k}}\rangle$$

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

$$= e^{+i\vec{k}\cdot\vec{t}}\, T|\psi_{n\vec{k}}\rangle = e^{+i\vec{k}\cdot\vec{t}} |\varphi\rangle$$

$|\varphi\rangle$ has crystal momentum $-\vec{k}$

Time-reversal invariant Momenta (TRIMs):

$\vec{k} \equiv -\vec{k}$ modulo a reciprocal lattice vector

$\vec{k} = \frac{1}{2}(n\vec{b}_1 + m\vec{b}_2 + l\vec{b}_3)$ $\quad \vec{b}_i$ primitive reciprocal lattice

$$T^2 = \bar{E}$$

vectors

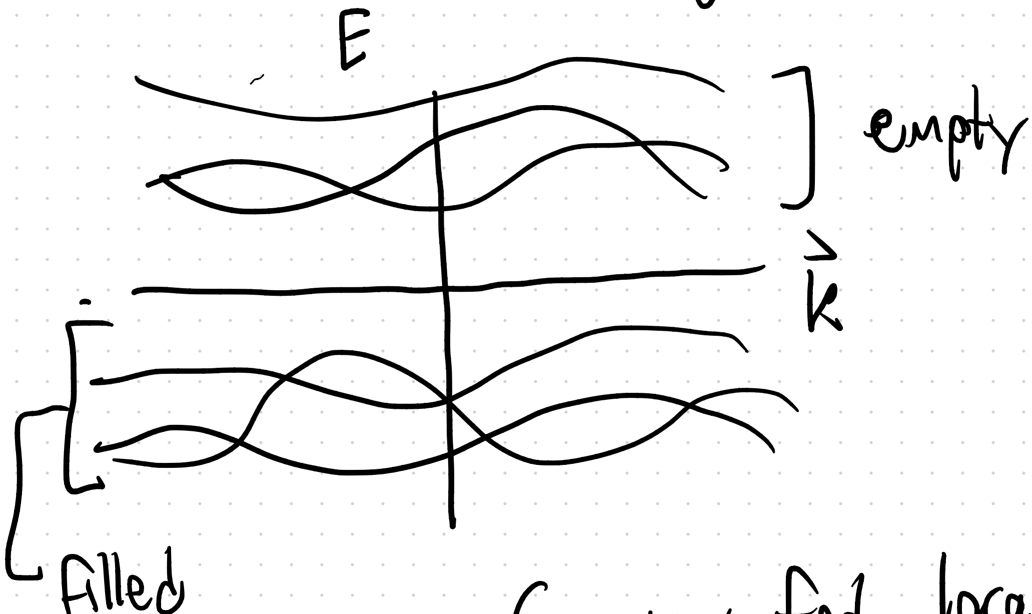
$n, m, l \in \{0, 1\}$

Two Stories:

① Hamiltonian invariant under space group G
→ Bloch's theorem → delocalized eigenstates

② "Chemistry" approach - solids are built out of atoms → atoms brought together and bond

2 → 1 Write down Schrödinger eqn, turn crank, get eigenstates



$|\psi_{nk}\rangle$, E_{nk}

Can we find localized functions made up of the occupied $|\psi_{nk}\rangle$

i.e. where do the electrons in an insulator live?

To address this, look at the position operator

$$\langle \psi_{n\vec{k}} | \vec{x} | \psi_{m\vec{k}'} \rangle = \int d^3x \, \psi^*_{nk}(\vec{x}) \, \vec{x} \, \psi_{mk'}(\vec{x})$$

Problem - $\psi_{nk}(x)$ delocalized $\rightarrow$ this integral diverges

To deal with this, we take continuum normalization convention

$$\langle \psi_{n\vec{k}} | \psi_{mk'} \rangle = \frac{(2\pi)^3}{v} \delta_{nm} \delta(\vec{k} - \vec{k}')$$

$v = |e_1 \cdot (\vec{e}_2 \times \vec{e}_3)|$ - volume of the unit cell

$|\psi_{n\vec{k}+G}\rangle = |\psi_{n\vec{k}}\rangle$ for G a reciprocal lattice vector

$$\sum_{\vec{t}} e^{i(k-k')\cdot\vec{t}} = \frac{(2\pi)^3}{v} \sum_G \delta(\vec{k} - \vec{k}' + G)$$

$$= \frac{(2\pi)^3}{v} \delta(\vec{k} - \vec{k}')$$

$$\langle \psi_{nk} | \psi_{mk'} \rangle = \int d^3x \, \psi^*_{nk}(x) \psi_{mk'}(x) \qquad \vec{x} = \vec{t} + \vec{y}$$

$\vec{y} \in$ primitive unit cell

$$= \sum_{\vec{t}} \int_{\text{cell}} d^3y \, \psi^*_{nk}(\vec{t}+\vec{y}) \psi_{mk'}(\vec{t}+\vec{y})$$

$$= \sum_{\vec{t}} \int_{\text{cell}} d^3y \, e^{i\vec{t}\cdot k'} e^{-i\vec{t}\cdot k} \psi^*_{nk}(y) \psi_{mk'}(y)$$

$$= \frac{(2\pi)^3}{v} \delta(k-k') \int_{\text{cell}} d^3y \, \psi^*_{nk}(y) \psi_{mk}(y)$$

$$= \frac{(2\pi)^3}{v} \delta(k-k') \int_{\text{cell}} d^3y \, u^*_{nk}(y) \, u_{mk}(y)$$

$$\psi_{nk}(x) = e^{ik\cdot x} u_{nk}(x)$$

Our normalization convention is

$$\langle u_{nk} | u_{mk} \rangle_{\text{cell}} = \int_{\text{cell}} d^3y \, u^*_{nk}(y) \, u_{mk}(y) = \delta_{nm}$$

Now lets compute $\langle \psi_{nk} | x^\mu | \psi_{mk'} \rangle \quad \mu = x, y, z$

$$= \int d^3x \, \psi^*_{nk}(\vec{x}) \, x^\mu \, \psi_{mk'}(\vec{x})$$

$$= \int d^3x \, x^\mu e^{i(k'-k)\cdot\vec{x}} \, u^*_{nk}(x) \, u_{mk'}(x)$$

$$= \int d^3x \, i \frac{\partial}{\partial k_\mu} \left[e^{i(k'-k)\cdot\vec{x}} \right] u^*_{nk}(x) \, u_{mk'}(x)$$

$$= i \frac{\partial}{\partial k_\mu} \left[\int d^3x \, e^{i(k'-k)\cdot x} \, u^*_{nk}(x) \, u_{mk'}(x) \right]$$

$$-i\int d^3x\, e^{i(k'-k)\cdot\vec{x}}\,\frac{\partial u^{*}_{nk}}{\partial k_\mu}(x)\, u_{mk'}(x) \qquad \vec{x}=t+y$$

$$= i\left(\frac{(2\pi)^3}{v}\right)\frac{\partial}{\partial k_\mu}\delta(k-k')\delta_{nm}$$

$$-i\sum_{\vec{t}} e^{i\vec{t}\cdot(k'-k)}\int_{\text{cell}} dy\, e^{i(k'-k)\cdot y}\,\frac{\partial u^{*}_{nk}(y)}{\partial k_\mu}\, u_{mk'}(y)$$

$$= i\left(\frac{(2\pi)^3}{v}\right)\left[\frac{\partial}{\partial k_\mu}\delta(k-k')\delta_{nm} + \delta(k-k')\right)\int_{\text{cell}} dy\; u^{*}_{nk}(y)\,\frac{\partial u_{mk}}{\partial k_\mu}$$

$$= \frac{(2\pi)^3}{V}\left[i\delta_{nm}\frac{\partial}{\partial k_\mu}\delta(k-k') + A_\mu^{nm}(k)\,\delta(k-k')\right]$$

$$A_\mu^{nm}(k) = i\int_{\text{cell}} dy\; u_{nk}^*(y)\frac{\partial u_{mk}}{\partial k_\mu} = i\left\langle u_{nk}\middle|\frac{\partial u_{mk}}{\partial k_\mu}\right\rangle_{\text{cell}}$$

Berry connection

To get intuition, lets consider a wave packet

$$|f\rangle = \sum_m \frac{V}{(2\pi)^3}\int d^3k' \, f_{mk'} \, |\psi_{mk'}\rangle$$

$$\langle \psi_{nk} | x^\mu | f \rangle = \frac{V}{(2\pi)^3}\sum_m \int d^3k' \, f_{mk'} \, \langle \psi_{nk} | x^\mu | \psi_{mk'} \rangle$$

$$= \int d^3k' \sum_m \left(i\delta_{nm} \frac{\partial}{\partial k_\mu} \delta(k-k') + A^{nm}_\mu (k) \delta(k-k') \right) f_{mk'}$$

$$= i \frac{\partial}{\partial k_\mu} f_{nk} + \sum_m A^{nm}_\mu (k) f_{mk}$$

Berry connection

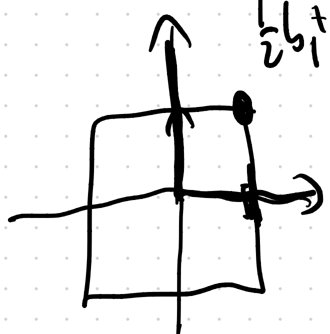
what we expect if $\vec{k}$ were "real" momentum

$$= i\left[D_\mu f\right]_{nk}$$

is a correction

$$D_\mu = \frac{\partial}{\partial k_\mu} - iA_\mu(k)$$

covariant derivative



2D $\vec{b}_1 = \hat{x}$

$\vec{b}_2 = \hat{y}$

$$C_{ZZ}\left(\frac{1}{2}b_1+\frac{1}{2}b_2\right) = -\frac{1}{2}b_1-\frac{1}{2}b_2$$

$$= \left(\frac{1}{2}b_1+\frac{1}{2}b_2\right)-\left(b_1+b_2\right)$$