Lecture 13

Recap: (1) Spin: electrons have spin $\frac{1}{2}$

2π rotation $\bar{E} \in SU(2)$ is different from the identity E

→ led us to introduce double space groups

$$G^d < \mathbb{R}^3 \rtimes Pin\_(3)$$

$$Pin\_(3) = \underbrace{SU(2)}_{\text{rotations}} \times \underbrace{\{E, I\}}_{\text{spatial inversion}}$$

Double group irreps ρ satisfy

$$\rho(\bar{E}) = \pm \rho(E)$$

+ - for spinless particles

→ ordinary space/point grp representations

⌣ for spin $\frac{1}{2}$ w/ SOC

② TRS represented as an antiunitary operator

$$T = B(T)\mathcal{K}$$

$$T^2 = \bar{E} \Rightarrow B(T)B^*(T) = \begin{cases} +Id & \text{for spinless} \\ -Id & \text{for spin-}\frac{1}{2} \end{cases}$$

Recall as group elements

$$Tg = gT \quad \text{for all } g \in G \quad \text{for space group } G$$

$\rho : G \to O(V)$ be an irrep of G

if T can be represented on the Hilbert space V

$$B(T)\mathcal{K}\rho(g) = \rho(g)\,B(T)\mathcal{K}$$

Ⓐ $\boxed{B(T)^{-1}\rho(g)\,B(T) = \rho^*(g)}$ For all group elements

Ⓑ $\boxed{B(T)\,B^*(T) = \rho(\bar{E})}$

Its <u>not</u> always possible to satisfy Ⓐ and Ⓑ

Example: point group $2^d = \{E, C_{2z}, \bar{E}, \bar{E}C_{2z}\}$

	E	$\bar{E}$	2	$2^d = \bar{E}C_{2z}$	
Γ_1	1	1	1	1	single-valued (spinless)
Γ_2	1	1	-1	-1	
$\bar{\Gamma}_3$	1	-1	$-i$	$+i$	double-valued (spin-$\frac{1}{2}$)
$\bar{\Gamma}_4$	1	-1	$+i$	$-i$	

for Γ_1 and Γ_2, we look for $B_{1/2}(T)\mathcal{K} \equiv \rho_{\Gamma_1/\Gamma_2}(T)$

$$B(T)B(T)^* = \mathbb{1}$$

$$B(T)\rho(C_{2z})^* = \rho(C_{2z})B(T)$$

$$\rightarrow \quad B(T) = \mathbb{1}$$

$$\rho(T) = \mathcal{K}$$

<u>But</u> for $\overline{\Gamma}_3$

$$B(T)\,\rho_{\overline{\Gamma}_3}(C_{2z})^* = \rho_{\overline{\Gamma}_3}(C_{2z})\,B(T)$$

$$B(T)(+i) = (-i)\,B(T)$$ No solution

$$\rho^*_{\overline{\Gamma}_3} \not\simeq \rho_{\overline{\Gamma}_3}$$

To make a time-reversal invariant representation, we need to add $\overline{\Gamma}_3$ and its conjugate $\overline{\Gamma}_3^* = \overline{\Gamma}_4$

$$\overline{\Gamma}_3\overline{\Gamma}_4 = \overline{\Gamma}_3 \oplus \overline{\Gamma}_4$$

$$\rho_{\bar{\Gamma}_3\bar{\Gamma}_4}(C_{2z}) = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\sigma_z$$

$$\boxed{\rho_{\bar{\Gamma}_3\bar{\Gamma}_4}(T) = i\sigma_y \mathcal{K}} = \begin{pmatrix} 0 & +1 \\ -1 & 0 \end{pmatrix}\mathcal{K}$$

$\bar{\Gamma}_3$ is a representation on $V_3 = \{|\uparrow\rangle\}$

$\bar{\Gamma}_4$ is a representation on $V_4 = \{|\downarrow\rangle\}$

"representations" w/ both unitary & antiunitary elements - <u>corepresentations</u>

$\bar{\Gamma}_3 \oplus \bar{\Gamma}_4$ is a reducible representation, but w/ TRS its an <u>irreducible correpresentation</u>

[on Billbao cryst. server (BCS)

" physically irreducible representations"

Hermann Mauguin TRS denoted by $1'$

eg $P432$ vs $P4321'$

Last point: How does TRS act on crystal momentum $\vec{k}$

Abstract: $\vec{k}$ labels irreps of Bravais lattice

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

- TRS maps reps to their conjugates
- $\rho_k^*(\vec{t}) = e^{+i k \cdot \vec{t}} = \rho_{-k}(\vec{t})$

$\Rightarrow$ TRS maps states @ $\vec{k}$ to states @ $-\vec{k}$

Concretely: $\mathcal{U}_{\vec{t}}|\psi_{nk}\rangle = e^{-ik\cdot\vec{t}}|\psi_{nk}\rangle$

$$\mathcal{U}_{\vec{t}}\left(T|\psi_{nk}\rangle\right) = T\,\mathcal{U}_{t}|\psi_{nk}\rangle = T e^{-ik\cdot t}|\psi_{nk}\rangle$$
$$= e^{+ik\cdot t}\left(T|\psi_{nk}\rangle\right)$$

if $-k \equiv k \mod \check{T}$ then $\rho_{-k} \cong \rho_{k}$

$\Rightarrow$ TRS is in the little group of $\vec{k}$

this occurs when

$$\vec{k} = \left\{ \frac{1}{2}\left(\sum_{i=1}^{3} n_i \vec{b}_i\right) \quad n_i = 0, 1 \right\}$$

$\vec{b}_i$ primitive reciprocal lattice vectors

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Time-reversal invariant momenta (TRIMs)

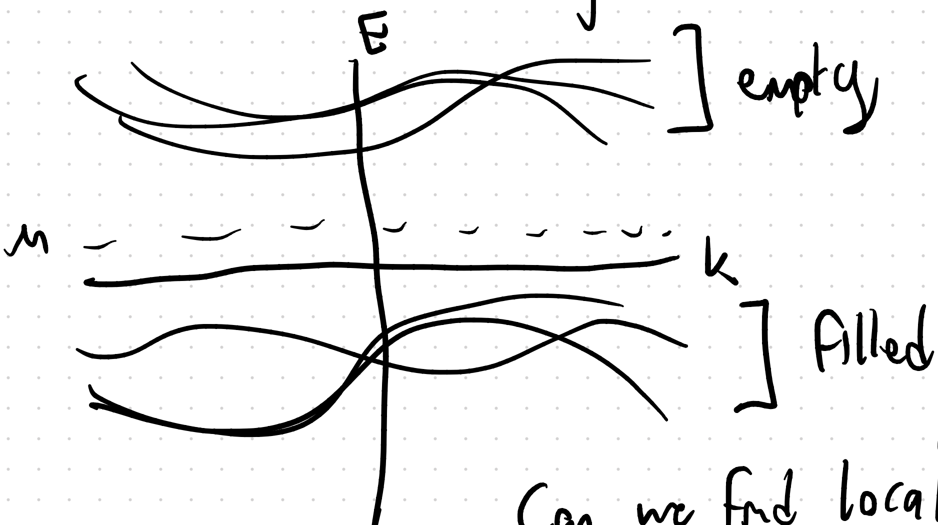
Two stories:

1. a Hamiltonian w/ space grp symmetries G → Bloch's theorem → a set of delocalized eigenstates

2. "Chemistry" approach: solids are built from atoms which "donates" some localized electrons to form bonds → band structure

② → ① is "easy": Write down Schrödinger eqn for all the atoms & all the electrons
→ turn the crank → energies & eigenstates

① → ② Say we have



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

Can we find localized "orbitals" made up of the occupied $\{|\psi_{nk}\rangle\}_{n=1}^{N_{occ}}$

- Where do the electrons live?

We can start by looking at the position operator $\vec{x}$

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

Problem: $\psi_{nk}(x)$ are delocalised - they are not normalizable

Continuum normalization convention

$$\underline{\langle \psi_{nk} | \psi_{mk'} \rangle} = \frac{(2\pi)^3}{v} \delta_{nm} \, \delta\left(\underline{\vec{k} - \vec{k}'}\right) \qquad k, k' \in BZ$$

$$\int_{BZ} d^3k = \frac{(2\pi)^3}{v}$$

$v = |\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)|$ - primitive unit cell volume

$|\psi_{nk+\vec{G}}\rangle = |\psi_{nk}\rangle$ for $\vec{G} \in \check{T}$

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

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

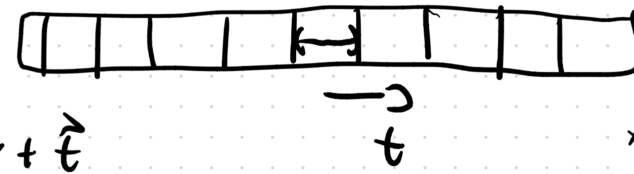
$$\underline{\langle \psi_{nk} | \psi_{mk'} \rangle} = \frac{(2\pi)^3}{v} \delta_{nm} \delta(\underline{\vec{k}-\vec{k}'})$$

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

$\downarrow$ Bloch's theorem $\psi_{nk}(x) = e^{ik\cdot x} u_{nk}(\vec{x})$

$u_{nk}(\vec{x}+\vec{t}) = u_{nk}(x)$

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



$$\vec{x} = \vec{y} + \vec{t}$$

$$= \sum_{\vec{t}} \int_{cell} dy\, e^{-i(k-k')\cdot(\vec{y}+\vec{t})}\, u^*_{nk}(\vec{y})\, u_{mk'}(\vec{y})$$

$$= \frac{(2\pi)^3}{v}\left[\int_{cell} dy\, u^*_{nk}(y)\, u_{mk}(y)\, \cancel{e^{-i(k-k')\cdot y}}\right]\delta(k-k')$$

$$\boxed{\text{Continuum normalization} \equiv \int_{cell} dy\, u^*_{nk}(y)\, u_{mk}(y) = \delta_{nm} \equiv \langle u_{nk} | u_{mk} \rangle}$$

Now:

$$\mu = x, y, z$$

$$\langle \psi_{nk} | x^{\mu} | \psi_{mk'} \rangle = \int d^3x \; x^{\mu} \psi^{*}_{nk}(x) \psi_{mk'}(x)$$

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

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

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

$$= i \frac{(2\pi)^3}{v} \delta_{nm} \frac{\partial}{\partial k^{\mu}} \delta(k-k') - i \sum_{t} e^{-i(k-k')\cdot \vec{t}} \int_{\text{cell}} dy \; e^{-i(k-k')\cdot y} \frac{\partial u^{*}_{nk}(y)}{\partial k^{\mu}} u_{mk'}(y)$$

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

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

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

<u>Berry connection</u>

to get intuition, consider a wavepacket

$$|f\rangle = \frac{v}{(2\pi)^3}\int dk' \sum_{n=1}^{N_{occ}} f_{mk'}|\psi_{mk'}\rangle$$

$$\langle \psi_{nk}|x^\mu|f\rangle = \frac{v}{(2\pi)^3}\int dk' \sum_{m=1}^{N_{occ}} f_{mk'}\langle \psi_{nk}|x^\mu|\psi_{mk'}\rangle$$

$$= \int dk' \sum_{m=1}^{N_{occ}} f_{mk'} \left(i \delta_{nm} \frac{\partial}{\partial k^\mu} \delta(k-k') + A_\mu^{nm}(k) \delta(k-k') \right)$$

$$= i \frac{\partial f_{nk}}{\partial k^\mu} + \sum_{m=1}^{N_{occ}} A_\mu^{nm}(k) f_{mk} = i [D_\mu f]_{nk}$$

what you get for position matrix elements if k were "real" momentum

correction due to the Berry connection

$$D_\mu = \frac{\partial}{\partial k_\mu} \delta_{nm} - i A_\mu(k)$$

"covariant derivative"

$$|\psi_{nk}\rangle \to e^{i\phi(k)} |\psi_{nk}\rangle$$