Lecture 14

Reminder: HW 2 is due today!

Last time: Time-reversal symmetry

- As a symmetry operation

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

- Wigner's theorem: T has to be represented as an antiunitary operator

→ corepresentation $\rho: G \to \{$unitary and antiunitary operators on $V\}$

$$\rho(T) = B(T)K$$

unitary

$$B(T)\,B^*(T) = \rho(\bar{E}) = \begin{cases} +\mathrm{Id} & \text{integer spin} \\ -\mathrm{Id} & \text{half-integer spin} \end{cases}$$

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

Start w/ $|\psi_{nk}\rangle$ $\qquad$ $\vec{t} \in$ Bravais lattice

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

what crystal momentum does $T|\psi_{nk}\rangle$ have?

$$U_{\vec{t}}\,T|\psi_{nk}\rangle = T\left(U_{\vec{t}}\,|\psi_{nk}\rangle\right)$$ (T commutes w/ all spatial symmetries)

$$= T\left(e^{-i\vec{k}\cdot\vec{t}}\,|\psi_{nk}\rangle\right)$$

$$= \left(e^{-i\vec{k}\cdot\vec{t}}\right)^{*} T|\psi_{nk}\rangle$$

$$= e^{-i(-k)\cdot\vec{t}}\, T|\psi_{nk}\rangle$$

$T|\psi_{nk}\rangle$ has crystal momentum $-\vec{k}$

If $-k \equiv k$ mod a reciprocal lattice vector, then $\overline{\text{TRS}}$ is in the little group G_k

$$\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$$

$$-\vec{k} = -k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$$

$$k - (-k) = 2k_1\vec{b}_1 + 2k_2 b_2 + 2k_3\vec{b}_3$$

when $k_i = \frac{n_i}{2}$ then $k = -\vec{k}$

$n_i = 0, 1$

8 $\underbrace{\text{time-reversal invariant momenta}}_{\text{TRIM}}$ in the BZ

Two stories

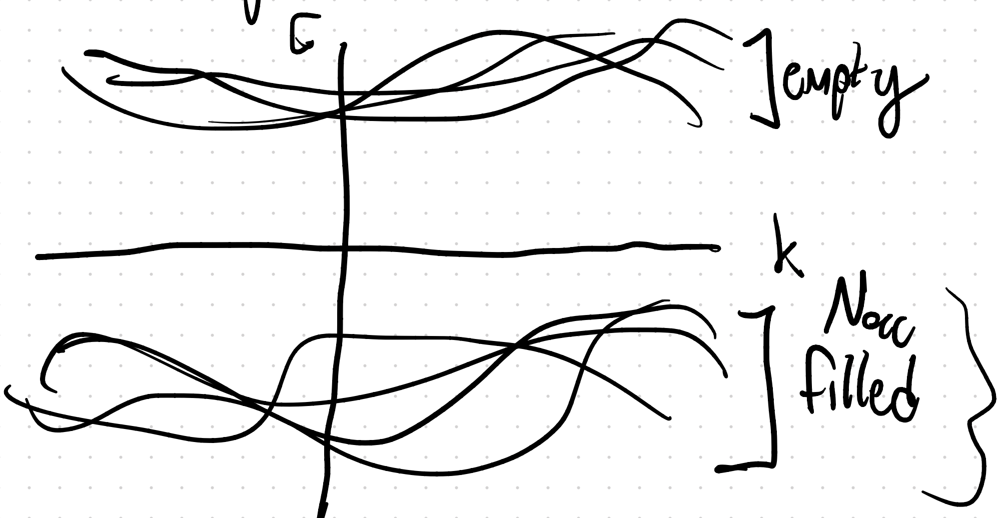
① A Hamiltonian w/ space grp G →
Bloch's theorem → a set of delocalized
$\psi_{nk}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{nk}(\vec{r})$

② "Chemistry" approach: start w/ atoms,
build a crystal, atoms "donate" localized
e^-'s to form bonds → band structure

② → ① straightforward: write down Schrödingers eqn for all atoms & electrons, → turn crank → energies and eigenstates

Can we go from ① → ②

Say we have an insulator



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

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

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

P - projection operator onto N_{occ} filled states

$$P|\psi_{nk}\rangle = \begin{cases} |\psi_{nk}\rangle & \text{if } n = 1, \dots, N_{occ} \\ 0 & \text{otherwise} \end{cases}$$

Projected position operator $P\vec{x}P$

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

Problem: $\psi_{nk}(x)$ not normalizable.

Continuum normalization convention

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

v - volume of the primitive unit cell

$|\vec{t}_1 \cdot (\vec{t}_2 \times \vec{t}_3)|$

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

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

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

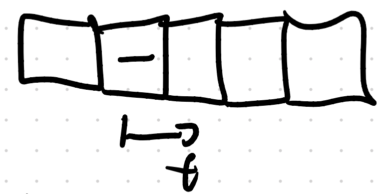
$$\int d^3x \, |\psi_{nk}(x)|^2 = \underline{\int d^3x \, |u_{nk}(x)|^2}$$

$$\int d^3x\, \psi^\dagger_{nk}(x)\, \psi_{mk'}(x) = \frac{(2\pi)^3}{v}\, \delta(k-k')\, \delta_{nm}$$

$$\parallel$$

$$\int d^3x\, e^{-ik\cdot x}\, u^\dagger_{nk}(x)\, e^{ik'\cdot x}\, u_{mk'}(x)$$

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



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

$$= \sum_t \int_{cell} d^3y\, e^{i(k'-k)\cdot t} \left[e^{i(k'-k)\cdot y}\, u^\dagger_{nk}(y\cancel{+t})\, u_{mk'}(y\cancel{+t}) \right]$$

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

continuum normalization: $\int_{cell} d^3y\, u^*_{nk}(y)\, u_{mk}(y) = \delta_{nm}$

$$\parallel$$

$$\langle u_{nk} | u_{mk} \rangle_{cell}$$

$\mu = 1, 2, 3$

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

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

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

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

$$= i \frac{\partial}{\partial k^\mu}\left(\frac{(2\pi)^3}{v}\delta(k-k')\delta_{nm}\right) - i \sum_{t\in T}\int_{cell} d^3y \, e^{-i(k-k')\cdot t} e^{-i(k-k')\cdot y} \frac{\partial u^*_{nk}(y)}{\partial k^\mu} u_{mk'}(y)$$

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

$$= \frac{(2\pi)^3}{v}\left[i\delta_{nm}\frac{\partial}{\partial k^\mu}\delta(k-k') + \delta(k-k')A^{nm}_\mu(\vec{k})\right] = \langle \psi_{nk} | R_x{}^\mu P | \psi_{mk'} \rangle$$

$$A^{nm}_{\mu}(k) = i\int_{cell} d^3y\; u^{*}_{nk}(y)\,\frac{\partial u_{mk}(y)}{\partial k^{\mu}} \equiv i\left\langle u_{nk}\middle|\frac{\partial u_{mk}}{\partial k^{\mu}}\right\rangle_{cell}$$

Berry connection

$$P = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle\langle\psi_{nk}|$$

Lets take a wavepacket $|f\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle f_{n\vec{k}}$

$$P x^{\mu} P|f\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle\langle\psi_{nk}|x^{\mu}|f\rangle$$

$$\sum_{m=1}^{N_{occ}} \int d^3k' \left[\frac{V}{(2\pi)^3}\right]^{2} \int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle\langle\psi_{nk}|x|\psi_{mk'}\rangle f_{mk'}$$

$$= \frac{V}{(2\pi)^3}\int d^3k' \int d^3k \sum_{n,m=1}^{N_{occ}} |\psi_{nk}\rangle \left(i\delta_{nm}\frac{\partial}{\partial k^\mu}\delta(k-k') + A_\mu^{nm}\delta(k-k')\right) f_{mk'}$$

$$= \frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle \underbrace{\left(i\frac{\partial f_{nk}}{\partial k^\mu} + \sum_m A_\mu^{nm}(k) f_{mk}\right)}$$

$$\frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle \left[iD_\mu f\right]_{nk} \qquad D_\mu = \frac{\partial}{\partial k^\mu} - iA_\mu(k)$$

covariant derivative

on wavepackets: PxP acts like a covariant derivative

Why "Covariant": Change of basis $|\psi'_{nk}\rangle = \sum_{m=1}^{N_{occ}} |\psi_{mk}\rangle U_{mn}(k)$

$N_{occ} \times N_{occ}$ unitary matrix

$U_{mn}(k+G) = U_{mn}(k)$

$$P' = \frac{v}{(2\pi)^3} \int d^3k \sum_{n=1}^{N_{occ}} |\psi'_{nk}\rangle\langle\psi'_{nk}|$$

$$= \frac{v}{(2\pi)^3} \int d^3k \sum_{m,l,n=1}^{N_{occ}} |\psi_{mk}\rangle \underbrace{U_{mn}(k) U^*_{ln}(k)}_{\delta_{ml}} \langle\psi_{lk}|$$

$= P \leftarrow$ P is invariant under $U(N_{occ})$ basis transformations

Transformation of wavepackets:

$$|f\rangle = \frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} f_{nk}|\psi_{nk}\rangle = \frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} f'_{nk}|\psi'_{nk}\rangle$$

$$\rightarrow \boxed{\vec{f}'_k = U^\dagger(k)\vec{f}_k}$$

$$|\psi'_{nk}\rangle = \sum_{m=1}^{N_{occ}} |\psi_{mk}\rangle U_{mn}(k)$$

$$\downarrow$$

$$|u'_{nk}\rangle = \sum_{m=1}^{N_{occ}} |u_{mk}\rangle U_{mn}(k)$$

Berry connection:

$$A^{(nm)}_\mu(k) = i\langle u'_{nk}|\frac{\partial}{\partial k^\mu} u'_{mk}\rangle$$

$$= i \sum_{l,p=1}^{N_{occ}} U^{\dagger}_{nl}(k) \langle u_{lk} | \frac{\partial}{\partial k^{\mu}} \left(|u_{pk}\rangle U_{pm}(k) \right)$$

$$= [U^{\dagger} A_{\mu} U]^{nm} + i \left[U^{\dagger} \frac{\partial}{\partial k_{\mu}} U \right]^{nm}$$ ← transformation law for a non-abelian gauge field

$$[D_{\mu} \vec{f}]'_{nk} = U^{\dagger} D_{\mu} \vec{f}$$

$$= U^{\dagger} D_{\mu} [U f']$$

$$= U^{\dagger} \left(\frac{\partial}{\partial k^{\mu}} (U f') - i A_{\mu} U f' \right)$$

$$= \frac{\partial f'}{\partial k^\mu} + U^\dagger \frac{\partial U}{\partial k^\mu} f' - i U^\dagger A_\mu U f'$$

$$= \frac{\partial f'}{\partial k^\mu} - i A'_\mu f' = D'_\mu \vec{f}'$$

D_μ is covariant under basis transformations

Given our occupied states - where do e^-'s in this insulator "line": what values of position could we find in a measurement of $P\hat{x}P$?

→ Eigenstates and Eigenvalues of $P\hat{x}P$

$$P x^\mu P |f\rangle = \lambda |f\rangle$$

$$\frac{V}{(2\pi)^3} \int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle [i D_\mu f]_{nk} = \frac{V}{(2\pi)^3} \int d^3k \, |\psi_{nk}\rangle \lambda f_{nk}$$

$$\boxed{\begin{gathered} i D_\mu f = \lambda f \\ f_{nk+G} = f_{nk} \end{gathered}}$$