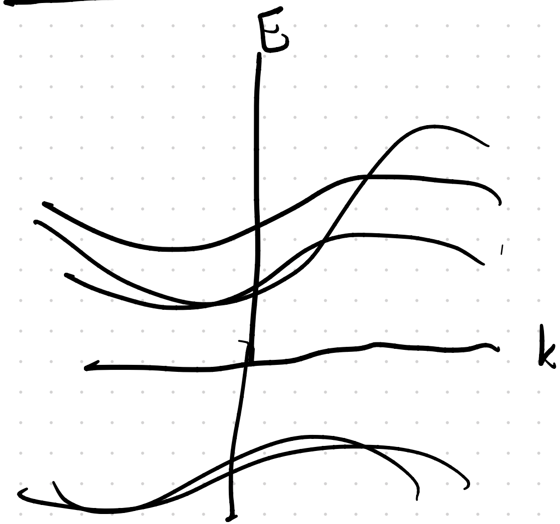
Lecture 14

Recap:



Energies E_{nk}

eigenstates $|\psi_{nk}\rangle = e^{ik\cdot x}|u_{nk}\rangle$

$$\langle \psi_{nk}|X^{\mu}|\psi_{mk'}\rangle = \frac{(2\pi)^3}{v}\left[i\delta_{nm}\frac{\partial}{\partial k_{\mu}}\delta(k-k') + A_{\mu}^{nm}(k)\,\delta(k-k')\right]$$

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

wave packet $|f\rangle = \sum_{nk} f_{nk} |\psi_{nk}\rangle$

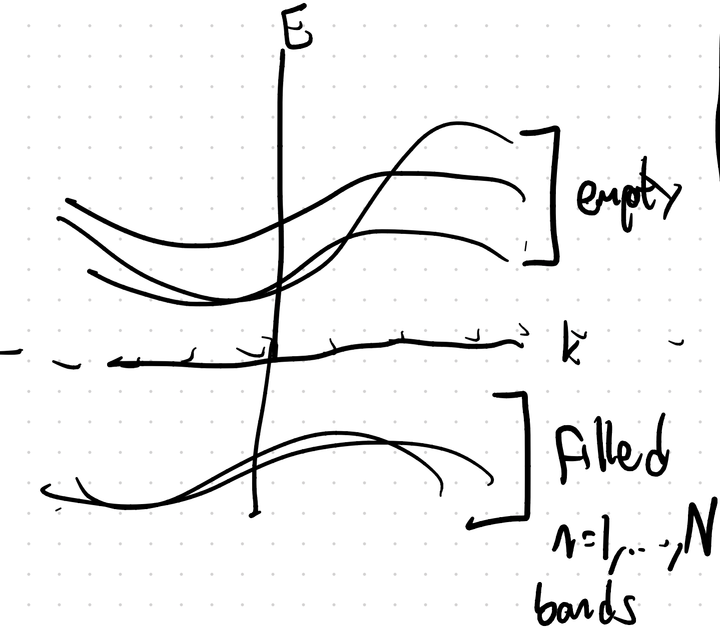
$$x^\mu |f\rangle = \sum |\psi_{nk}\rangle [iD_\mu f]_{nk}$$

$$[D_\mu f]_{nk} = \frac{\partial f_{nk}}{\partial k_\mu} - \sum_m i A^{nm}_\mu f_{mk}$$ Covariant derivative

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

$$He^{i\vec{k}\cdot\vec{x}}|u_{nk}\rangle = E_{nk} e^{ik\cdot x}|u_{nk}\rangle$$

$$\boxed{H(k)} = e^{-ik\cdot x} H e^{ik\cdot x}$$



$$E_\mu(t) = -\frac{\partial a_\mu}{\partial t}$$ electromagnetic vector potential

$$a_\mu = -E_\mu^{(0)} t$$

$$k \to k + E_\mu^{(0)} t$$

Zak, PRL 62, 2747 (1989)

$$P = \frac{v}{(2\pi)^3} \int d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle\langle\psi_{nk}|$$ projector onto filled bands

$Px^\mu P$ - projected position operator

, f $|f\rangle = \frac{V}{(2\pi)^3}\sum_{m=1}^{N}\int d^3k \, |\psi_{mk}\rangle f_{mk}$ is a

wavepacket made out of occupied states

$$P x^\mu P|f\rangle = \int \frac{V}{(2\pi)^3} d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle \left(i \frac{\partial f_{nk}}{\partial k_\mu} + \sum_{m=1}^{N} A_\mu^{nm}(k) f_{mk} \right)$$

$$= \int \frac{V}{(2\pi)^3} d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle \left[i D_\mu f_{nk} \right]$$

Why do we say D_μ is covariant?

Change of basis $|\psi'_{nk}\rangle = \sum_{m=1}^{N} |\psi_{mk}\rangle U_{mn}(k)$

$N \times N$ unitary matrix $U_{mn}(k+G) = U_{mn}(k)$ for $G \in$ reciprocal lattice

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

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

$$= \frac{V}{(2\pi)^3} \int d^3k \sum_{n,l,m=1}^{N} |\psi_{mk}\rangle\langle\psi_{lk}| \, U_{mn}(k) U^\dagger_{nl}(k)$$

$$= P$$

Projection operator is <u>invariant</u> under a $U(N)$ change of basis

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

$$\Rightarrow \boxed{f'_{nk} = \sum_{m=1}^{N} U^{\dagger}_{nm}(k) f_{mk}}$$

Berry connection:

$$A'^{nm}_{\mu}(k) = i\left\langle u'_{nk} \middle| \frac{\partial u'_{mk}}{\partial k_{\mu}} \right\rangle_{cell}$$

$$= i\left(\sum_{\ell=1}^{N} U^{\dagger}_{n\ell}(k) \langle u_{\ell k}| \frac{\partial}{\partial k_{\mu}}\left(\sum_{p=1}^{N} |u_{pk}\rangle U_{pm}(k)\right)\right)$$

$$= [U^{\dagger} A_{\mu}(k) U]^{nm} + i \sum_{\ell,p=1}^{N} U^{\dagger}_{n\ell}(k) \overbrace{\langle u_{\ell k} | u_{pk}\rangle_{cell}}^{\delta_{\ell p}} \frac{\partial U_{pm}}{\partial k_{\mu}}$$

$$= \left[U^\dagger(k) A_\mu(k) U(k) + i U^\dagger \frac{\partial}{\partial k_\mu} U \right]^{nm}$$

non-Abelian gauge transformation

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

$$= U^\dagger D_\mu (U f')$$

$$= \left(\frac{\partial}{\partial k_\mu} - i A'_\mu \right) f'$$

$$= D'_\mu f'$$

Ex: one band $|\psi_{1k}\rangle = |\psi_1\rangle$

$$U = e^{i\theta(k)}$$

$$A'_\mu = A_\mu + i e^{-i\theta(k)} \frac{\partial}{\partial k_\mu} e^{i\theta(k)}$$

$$= A_\mu - \partial_\mu \theta$$

$D_\mu \vec{f}$ transforms like $\vec{f}$ under gauge transformations

(changes of basis)

Eigenstates and Eigenvalues $P x_\mu P$

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

$$\Rightarrow \quad i D_\mu \vec{f} = \lambda \vec{f}$$

Simple case: One occupied band $|\psi_k\rangle$ $\quad P = \frac{v}{(2\pi)^3} \int d^3k \, |\psi_k\rangle\langle\psi_k|$

$$|f\rangle = \frac{v}{(2\pi)^3} \int d^3k \, f_k |\psi_k\rangle$$

$$iD_\mu f_k = i\frac{\partial f_k}{\partial k_\mu} + A_\mu(k) f_k = \lambda f_k$$

$\vec{b}_\mu$ - primitive reciprocal lattice vectors

derivatives wrt reduced coordinates

$$x^\mu = \frac{1}{2\pi}\vec{b}_\mu \cdot \vec{X}$$

reciprocal lattice vector

$$\vec{k} = \sum_{\nu=1}^{3} k_\nu \vec{b}_\nu \left(\frac{1}{2\pi}\right) \qquad k_\mu \in [-\pi, \pi]$$

$$\vec{k} = k_\mu \vec{b}_\mu \frac{1}{2\pi} + \vec{k}_\perp$$

Ansatz: $f(k_\mu, \vec{k}_\perp) = g(k_\mu, \vec{k}_\perp, k_0)\, e^{i\int_{k_0}^{k_\mu} dk_\mu' A_\mu(k_\mu', \vec{k}_\perp)}$

$$i\frac{\partial g(k_\mu,\vec{k}_\perp,k_0)}{\partial k_\mu} = \lambda g(k_\mu,k_\perp,k_0)$$

$$g(k_\mu,k_\perp,k_0) = e^{-i\lambda(k_\perp)k_\mu} f(k_\perp,k_0)$$

$$\boxed{f(k_\mu,k_\perp,k_0) = e^{i\left[\int_{k_0}^{k_\mu} dk_\mu A_\mu(k_\mu',k_\perp) - \lambda(k_\perp)k_\mu\right]} f(k_\perp,k_0)}$$

Periodicity: $f(k_\mu+2\pi,k_\perp,k_0) = f(k_\mu,k_\perp,k_0)$

$$\parallel$$

$$e^{i\int_{k_\mu}^{k_\mu+2\pi} dk_\mu A_\mu(k_\mu',k_\perp) - 2\pi i\lambda(k_\perp)} f(k_\mu,k_\perp,k_0)$$

$$\int_0^{2\pi} dk_\mu A_\mu(k_\mu', k_\perp) = \varphi(k_\perp) \quad \text{- Berry phase}$$

$$\downarrow$$

$$\boxed{\lambda(k_\perp) = \frac{1}{2\pi}\varphi(k_\perp) + n}$$

$$|W_{n k_\perp}\rangle = \frac{1}{2\pi}\int_{k_0}^{2\pi + k_0} dk_\mu \times$$

$$|\psi_{\vec{k}}\rangle \times e^{i\left[\int_{k_0}^{k_\mu} dk_\mu' A(k) - \frac{k_\mu \varphi(k_\perp)}{2\pi} - k_\mu n\right]}$$

$$A_\mu(k) = \left\langle u_k \middle| \frac{\partial u_k}{\partial k_\mu} \right\rangle$$

$$|\psi_k\rangle = |\psi_{k+2\pi}\rangle$$

$$\cancel{e^{ikx}} |u_k\rangle = \cancel{e^{ikx}} e^{i 2\pi \cdot x} |u_{k+2\pi}\rangle$$

$$A(k+2\pi) = \langle u_{k+2\pi} | \frac{\partial}{\partial k_\mu} u_{k+2\pi} \rangle$$

$$= \langle u_k | \cancel{e^{2\pi i x}} \frac{\partial}{\partial k_\mu} \left(\cancel{e^{2\pi i x}} | u_k \rangle \right)$$

$$= A(k)$$

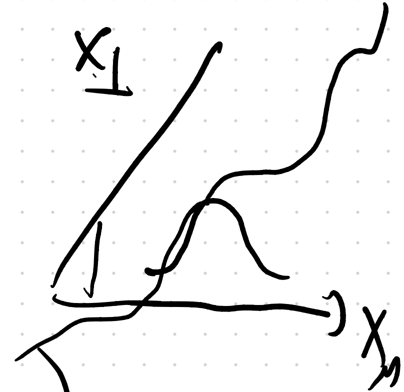
$$|W_{nk_\perp}\rangle = \frac{1}{2\pi} \int_{k_0}^{k_0+2\pi} dk_\mu \, |\varphi_{\vec{k}}\rangle \, e^{i\left[\int_{k_0}^{k_\mu} dk_\mu' A_\mu(k_\mu', k_\perp) - \frac{k_\mu \varphi(k_\perp)}{2\pi} - n k_\mu\right]}$$

$$P x_\mu P |W_{nk_\perp}\rangle = \left(\frac{\varphi(k_\perp)}{2\pi} + n \right) |W_{nk_\perp}\rangle$$

Hybrid Wannier function

displacement relative to origin of that unit cell

unit cell index



The Berry phase $\frac{1}{2\pi}\int_0^{2\pi} dk_\parallel A_\parallel(k_\parallel, k_\perp)$ gives us (the fractional part of) the spectrum of $P x_\parallel P$

$$\langle W_{nk_\perp} | P x^2 P | W_{nk_\perp} \rangle = \langle W_{nk_\perp} | P x P x P | W_{nk_\perp} \rangle$$
$$+ \langle W_{nk_\perp} | P x (1-P) x P | W_{nk_\perp} \rangle$$

$$\frac{1}{2\pi}\vec{b}_\mu \cdot \left(t_1\vec{e}_1 + t_2\vec{e}_2 + t_3\vec{e}_3\right)$$

t_μ $\vec{e}_\mu$