Lecture 14

Announcements: - HW1 is graded, solutions are posted

- HW2 is due today
- HW3 will be posted tonight

Reminder: H w/ discrete translation symmetry

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

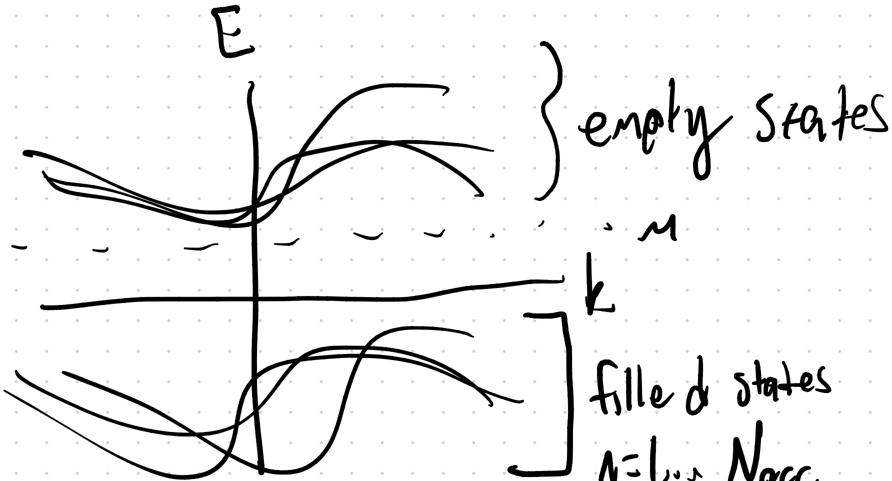
$$\langle\vec{r}|\psi_{nk}\rangle = e^{ik\cdot\vec{r}}\, u_{nk}(\vec{r}) \qquad u_{nk}(\vec{r}+\vec{t}) = u_{nk}(r)$$

$\forall \vec{t} \in$ Bravais lattice

$$\langle u_{nk}|u_{mk}\rangle = \int_{\text{cell}} dr\, u^*_{nk}(\vec{y})\, u_{mk}(\vec{y}) = \delta_{nm}$$

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

$$A^{nm}_\mu(k) = i\left\langle u_{nk} \middle| \frac{\partial u_{mk}}{\partial k^\mu}\right\rangle$$ is the Berry connection



$$\left(\prod_{n=1}^{N_{occ}} c^\dagger_{nk}\right)|0\rangle$$

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

projected position operator $Px^\mu P$

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

We can try to find localized states by looking for eigenfunctions of $P x^\mu P$

$$P x^\mu P |f\rangle \overset{?}{=} \lambda |f\rangle$$

wavepacket $\quad |f\rangle = \frac{V}{(2\pi)^3} \int d^3k' \sum_{m=1}^{N_{occ}} f_{mk'} |\psi_{mk'}\rangle$

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

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

$$[D_\mu F]_{nk} = \frac{\partial F_{nk}}{\partial k^\mu} - i \sum_{m=1}^{N_{occ}} A_\mu^{nm}(k) F_{mk}$$ Covariant derivative

Why do we call D covariant?

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

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

$U(k+\vec{G}) = U(\vec{k})$ where $\vec{G} \in \Upsilon$

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

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

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

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

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

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

Berry connection: $\quad |\psi_{nk}\rangle = e^{ik\cdot x}\,|u_{nk}\rangle$

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

$$A'^{nm}_{\mu}(k) = i\langle u'_{nk}|\frac{\partial u'_{mk}}{\partial k_\mu}\rangle = \sum_{l,p=1}^{N_{oc}} U^\dagger_{nl}\langle u_{lk}|\frac{\partial}{\partial k^\mu}\left(|u_{pk}\rangle U_{pm}(k)\right)$$

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

Now for the covariant derivative

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

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

$$= U^\dagger\left(\partial_\mu(Uf') - iA_\mu Uf'\right)$$

$$= \partial_\mu f' + U^\dagger \partial_\mu U f' - i U^\dagger A_\mu U f'$$

$$= \partial_\mu f' - i A'_\mu f'$$

$$= D'_\mu \tilde{f}' \rightarrow$$ $D_\mu f$ transforms like $\tilde{f}$ under basis transformations (gauge transformations)

Coordinates $\boxed{x_i} = \frac{1}{2\pi} \vec{b}_i \cdot \vec{x}$ $\quad \vec{b}_i$ - primitive reciprocal lattice vector

$$\vec{k} = \frac{1}{2\pi}\left(k_1 \vec{b}_1 + k_2 \vec{b}_2 + k_3 \vec{b}_3 \right) \qquad k_1, k_2, k_3, \ (-\pi, \pi]$$

$$x_i e^{i\vec{k}\cdot x} = -i \frac{\partial}{\partial k_i} e^{ik\cdot\vec{x}}$$

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

$$D_i f_{nk} = \frac{\partial f_{nk}}{\partial k_i} - i \sum_{m=1}^{N_{occ}} A_i^{nm}(k) f_{mk}$$

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

$$i \left[D_i f\right]_{nk} = \lambda f_{n\vec{k}}$$

Warmup for today $N_{occ} = 1$ $\quad P = \frac{V}{(2\pi)^3} \int d^3k \, |\psi_k\rangle\langle\psi_k|$

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

$$i D_i f = i \frac{\partial f(\vec{k})}{\partial k_i} + A_i(k) f(\vec{k}) = \lambda f(\vec{k})$$

$$\vec{k} = \frac{1}{2\pi} k_i \vec{b}_i + \sum_{j \neq i} \frac{k_j}{2\pi} \vec{b}_j$$

$$= \frac{1}{2\pi} k_i \vec{b}_1 + \vec{k}_\perp$$

ansatz:

$$f(k_i,\vec{k}_\perp) = g(k_i,k_\perp)e^{+i\int_{k_0}^{k_i} dk_i' A_i(k_i',\vec{k}_\perp)}$$

$$i\frac{\partial}{\partial k_i} g(k_i,k_\perp) = \lambda g(k_i,k_\perp)$$

$$g(k_i,k_\perp) = e^{-i\lambda k_i} C(k_\perp)$$

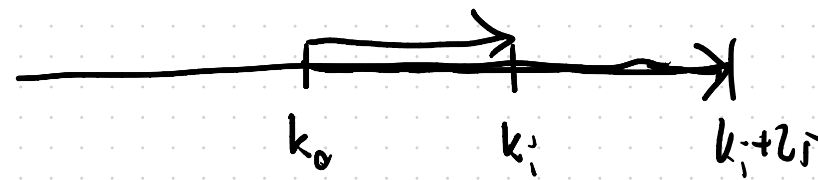
$$\boxed{\underline{f(k_i,k_\perp)} = C(k_\perp)e^{i\int_{k_0}^{k_i} dk_i' A_i(k_i',\vec{k}_\perp) - i\lambda k_i}}$$

Need to enforce periodicity:

$$f(k_i+2\pi, k_\perp) = f(k_i)$$

$$e^{i\int_{k_0}^{k_i+2\pi} dk_i' A_i(k_i', \vec{k}_\perp) - i\lambda(\cancel{k_i}+2\pi)} = e^{i\int_{k_0}^{k_i} dk_i' A_i(k_i', k_\perp) - i\cancel{\lambda k_i}}$$

$$e^{i2\pi\lambda} = e^{i\left[\int_{k_0}^{k_i+2\pi} dk_i' A_i(k_i', k_\perp) - \int_{k_0}^{k_i} dk_i' A_i(k_i', k_\perp)\right]}$$



$$e^{2\pi i\lambda} = e^{i\int_{k_i}^{k_i+2\pi} dk_i' A_i(k_i', k_\perp)}$$

Note $A_i(k_i+2\pi, k_\perp) = A_i(k_i, \vec{k}_\perp)$

$$A_i(k_i+2\pi, \vec{k}_\perp) = i\int_{\text{cell}} dy\, u^{(y)}_{k_i+2\pi, k_\perp} \frac{\partial}{\partial k_i} u^{(y)}_{k_i+2\pi, k_\perp}$$

$$|\psi_{k_j+2\pi}\rangle = |\psi_{k_j}\rangle$$

$$|u_k\rangle = e^{-ik\cdot x}|\psi_k\rangle \Rightarrow |u_{k_j+2\pi}\rangle = e^{-2\pi i x}|u_{k_j}\rangle$$

$$= A_i(k_j, k_\perp)$$

$$\int_{k_j}^{k_j+2\pi} dk_j' A_j(k_j, k_\perp) = \cancel{\int_{k_i}^{0} dk_i'} + \int_0^{2\pi} dk_i + \cancel{\int_{2\pi}^{k_j+2\pi} dk_j} A_i(k_j', \vec{k}_\perp)$$

$$= \int_0^{2\pi} dk_j A_i(k_i', \vec{k}_\perp) \equiv \varphi(k_\perp)$$

Berry phase

$$e^{2\pi i \lambda} = e^{i\varphi(k_\perp)}$$

$$\lambda_n(k_\perp) = \frac{\varphi(k_\perp)}{2\pi} + n \leftarrow P x_i P \text{ eigenvalues}$$

$n \in \mathbb{Z}$

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

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

Hybrid Wannier functions

Putting back units, $|W_{nk_\perp}\rangle$ is centered at

$$\vec{r}_n(k_\perp) = \left(\frac{\varphi(k_\perp)}{2\pi} + n\right)\vec{t}_i$$

displacement relative to the center of the unit cell

which unit cell $|W_{nk_\perp}\rangle$ is in

$$\boxed{\text{The Berry phase } \varphi(k_\perp) = \int_0^{2\pi} dk_i\, A_i(k_i, \vec{k}_\perp) \text{ gives the fractional part of the spectrum of } P x_i P}$$