

Lecture 22

Tight-binding approximation

$$|\Psi_{nk}\rangle \simeq \sum_{a=1}^N u_{nk}^a |\chi_{ak}\rangle$$

$$|\Psi_{k+\vec{G}}\rangle = |\Psi_{nk}\rangle$$

$$|\chi_{ak}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\vec{\tau}_a)} |\varphi_{\mathbf{R}}\rangle$$

$$|\chi_{ak+\vec{G}}\rangle = V_{ab}(\mathbf{G}) |\chi_{bk}\rangle$$

$$V(\mathbf{G}) = e^{i\mathbf{G}\cdot\vec{\tau}_a} \delta_{ab}$$

$$\vec{u}_{nk+\vec{G}} = V^\dagger(\mathbf{G}) \vec{u}_{nk}$$

$$H |\Psi_{nk}\rangle \simeq E_{nk} |\Psi_{nk}\rangle \quad \text{if}$$

$$h(\mathbf{k}) \vec{u}_{nk} = E_{nk} \vec{u}_{nk}$$

$$h^{ab}(k) = \langle \chi_{ak} | L_H | \chi_{bk} \rangle$$

given $g \in G$ s.t. $U_g^\dagger H U_g = H$ $g = \{\bar{g} | \vec{d}\}$

then $U_g | \chi_{ak} \rangle = | \chi_{b\bar{g}k} \rangle B_{ba}(\bar{g}) e^{-i\bar{g}k \cdot \vec{d}}$

$$B(\{E | \vec{E}\} \{ \bar{g} | \vec{d} \}) = B(\{ \bar{g} | \vec{d} \})$$

In the tight-binding limit $(\langle W_{aR} | \vec{x} | W_{bR'} \rangle = \tilde{T}_{ab} \delta_{RR'})$

$$A_m^{nm}(k) \simeq i \vec{u}_{nk}^\dagger \cdot \partial_m \vec{u}_{nk}$$

In particular, let's look at a "trivial" eigenstate

$$|\psi_{ak}^0\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |W_{a\mathbf{R}}\rangle$$

eigenstate of a Hamiltonian w/ no hopping

$$|\psi_{ak}^0\rangle = \sum_b u_{ak}^b |\chi_{bk}\rangle = \sum_{b\mathbf{R}} u_{ak}^b e^{i\mathbf{k}\cdot(\mathbf{R}+\vec{\Gamma}_b)} |W_{b\mathbf{R}}\rangle$$

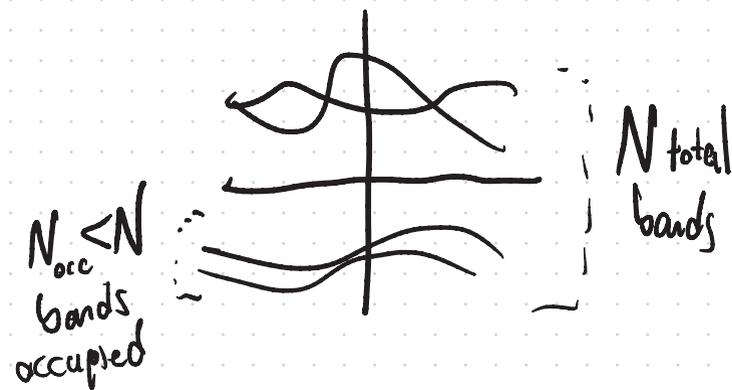
$$u_{ak}^b = \delta_a^b e^{-i\mathbf{k}\cdot\vec{\Gamma}_a}$$

$$A_{\mu}^{aa} = i u_{ak}^{\dagger} \partial_{\mu} u_{ak} = \vec{\Gamma}_a^{\mu}$$

$$\begin{aligned} h(\mathbf{k}) \vec{u}_{nk} &= E_{nk} \vec{u}_{nk} \\ \vec{u}_{nk} \rightarrow e^{i\mathcal{F}(\mathbf{k})} \vec{u}_{nk} &= \vec{u}'_{nk} \end{aligned}$$

Our Fourier-transform convention ensures that the f.b. Berry connection approximates the (projected) position operator

Let's look @ tight-binding Wilson loops



We can construct a

$$\sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} W_{\mathbf{aR}}(\vec{\mathbf{r}})$$

$\{E|\vec{\mathbf{t}}\}$

$$\sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} W_{\mathbf{aR}}(\vec{\mathbf{r}} - \vec{\mathbf{t}})$$

$$W_{\mathbf{aR}}(\vec{\mathbf{r}}) = W_{\mathbf{a0}}(\vec{\mathbf{r}} - \vec{\mathbf{R}})$$

t, b. projection operator

$$P_{ab}(k) = \sum_{n=1}^{N_{occ}} U_{nk}^a (U_{nk})^{\dagger b}$$

$$P_{ab}(k) U_{mk}^b = \sum_{n=1}^{N_{occ}} U_{nk}^a \left[(U_{nk})^{\dagger b} U_{mk}^b \right]$$

$$= \sum_{n=1}^{N_{occ}} U_{nk}^a U_{nk}^{\dagger} U_{mk} = \begin{cases} \vec{U}_{mk} & \text{if } m \text{ is occupied} \\ 0 & \text{if } m \text{ is unoccupied} \end{cases}$$

$$W_{k_{\parallel} \leftarrow 0}^{mm}(\vec{k}_{\perp}) = \vec{U}_{n_{k_{\parallel}, k_{\perp}}}^{\dagger} \cdot \prod_{k'_{\parallel} \leftarrow 0}^{k_{\parallel} \leftarrow 0} P(k'_{\parallel}, k_{\perp}) \cdot \vec{U}_{m0, k_{\perp}} = \mathcal{P} e^{i \int_0^{k_{\parallel}} \sum_{n, m} U_{nk}^{\dagger} \partial U_{mk}}$$

$$\sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} W_{a\mathbf{R}+\vec{t}}(\mathbf{r})$$

$$\mathbf{R}' = \mathbf{R} + \vec{t}$$

$$\sum_{\mathbf{R}'} e^{i\mathbf{k} \cdot (\mathbf{R}' - \vec{t})} W_{a\mathbf{R}'}(\mathbf{r}) = e^{-i\mathbf{k} \cdot \vec{t}} \psi_{ab}^{\circ}(\mathbf{r})$$

(t.b. - tight-binding)

$$i D_n^{(t.b.)} W = 0$$

Symmetries and the t.b. Wilson loop $g = \{\bar{g} | \vec{d}\}$

$$U_g |\chi_{ak}\rangle = |\chi_{b\bar{g}k}\rangle B_{ba}(\bar{g}) e^{-i\bar{g}k \cdot \vec{d}}$$

This is "passive" b/c symmetries act on basis fns $|\chi\rangle$

Active: $|\Psi_{nk}\rangle \rightarrow |\Psi'_{n\bar{g}k}\rangle = U_g |\Psi_{nk}\rangle$
 $= \sum_a U_{nk}^a U_g |\chi_{ak}\rangle$

$$= \sum_{ab} u_{nk}^a B_{ba}(\vec{g}) |\chi_{b\vec{g}k}\rangle e^{-i\vec{g}k \cdot \vec{d}}$$

$$u_{n\vec{g}k}^{b'} = B_{ba}(\vec{g}) e^{-i\vec{g}k \cdot \vec{d}} u_{nk}^a$$

Sewing matrix

$$B_k^{nm}(\vec{g}) = \vec{u}_{n\vec{g}k}^+ \vec{u}'_{m\vec{g}k}$$

$$= \vec{u}_{n\vec{g}k}^+ \cdot \left[B(\vec{g}) e^{-i\vec{g}k \cdot \vec{d}} \right] \cdot \vec{u}_{mk}$$

$$e^{i\vec{g}k \cdot \vec{d}} B_{ab}^+(\vec{g}) h_{bc}(\vec{g}k) B_{cd}(\vec{g}) e^{-i\vec{g}k \cdot \vec{d}} = h_{ad}(k)$$

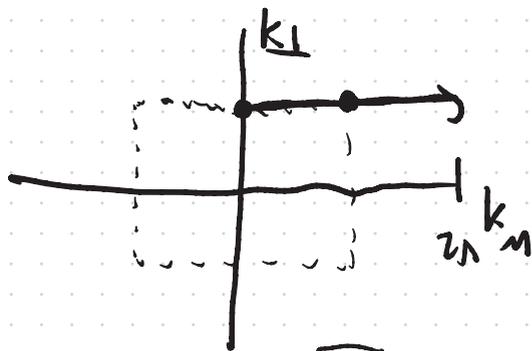
$$\Rightarrow P_{ab}(k) = \beta_{ac}^\dagger(g) P_{cd}(\bar{g}k) \beta_{db}(g)$$

Example: tight-binding Wilson loop w/ Inversion symmetry $g = \{\mathbb{I} | \vec{0}\}$

$$W_{2\pi\vec{e}_0}^{mn}(k_\perp) = U_{n, 2\pi, k_\perp}^\dagger \cdot \prod_{k'_\perp}^{2\pi\vec{e}_0} P(k'_\perp, k_\perp) \cdot U_{m, 0, k_\perp}$$

$$= \left(V^\dagger(2\pi) U_{n, 0, k_\perp} \right)^\dagger \cdot \prod_{k'_\perp}^{2\pi\vec{e}_0} P(k'_\perp, k_\perp) \cdot U_{m, 0, k_\perp}$$

$$= U_{n, 0, k_\perp}^\dagger \left[V(2\pi) \prod_{k'_\perp}^{2\pi\vec{e}_0} P(k'_\perp, k_\perp) \right] U_{m, 0, k_\perp}$$



$$= U_{n0, k_{\perp}}^{\dagger} \left[\prod_{k'_{\parallel}}^{2\pi \zeta - \pi} V(2\pi) P(k'_{\parallel}, k_{\perp}) \right] \left[\prod_{k''_{\parallel}}^{\pi \zeta - 0} P(k''_{\parallel}, k_{\perp}) \right] U_{m0, k_{\perp}}$$

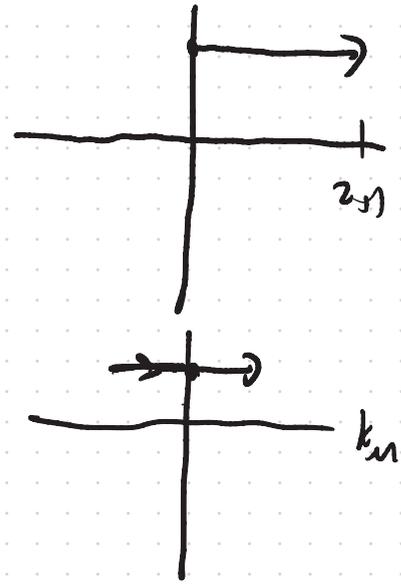
$$P(k'_{\parallel} + G, k_{\perp}) = V^{\dagger}(G) P(k'_{\parallel}, k_{\perp}) V(G)$$

$$= U_{n0, k_{\perp}}^{\dagger} \left[\prod_{k'_{\parallel}}^{0 \zeta - \pi} P(k'_{\parallel}, k_{\perp}) \right] U_{\ell \pi, k_{\perp}}^{\dagger} U_{\ell \pi, k_{\perp}}^{\dagger} \left[\prod_{k''_{\parallel}}^{\pi \zeta - 0} P(k''_{\parallel}, k_{\perp}) \right] U_{m0, k_{\perp}}$$

$$= W_{0 \leftarrow -\pi}(k_{\perp}) W_{\pi \leftarrow 0}(k_{\perp})$$

lets assume k_{\perp} is a TRIM

$$k_{\perp} = -k_{\perp} + G$$



$$\begin{aligned} P(k_{\parallel}, k_{\perp}) &= B^{\dagger}(\mathbf{I}) P(-k_{\parallel}, -k_{\perp}) B(\mathbf{I}) \\ &= B^{\dagger}(\mathbf{I}) P(-k_{\parallel}, k_{\perp} - G) B(\mathbf{I}) \\ &= B^{\dagger}(\mathbf{I}) V(G) P(-k_{\parallel}, k_{\perp}) V^{\dagger}(G) B(\mathbf{I}) \end{aligned}$$

$$\prod_{k_m}^{0 \leftarrow -\pi} P(k_m, k_{\perp}) = B^{\dagger}(\mathbb{I})V(G) \prod_{k_m}^{0 \leftarrow \pi} P(k_m, k_{\perp}) V^{\dagger}(G)B(\mathbb{I})$$

$$= B^{\dagger}(\mathbb{I})V(G) \left[\prod_{k_m}^{\pi \leftarrow 0} P(k_m, k_{\perp}) \right]^{\dagger} V^{\dagger}(G)B(\mathbb{I})$$

$$W_{0 \leftarrow -\pi} = u_{n0k_{\perp}}^{\dagger} \cdot B^{\dagger}(\mathbb{I})V(G) \left[\prod_k^{\pi \leftarrow 0} P(k_m, k_{\perp}) \right]^{\dagger} V^{\dagger}(G)B(\mathbb{I})u_{l-\pi k_{\perp}}$$

$$= \boxed{u_{n0k_{\perp}}^{\dagger} \cdot [B^{\dagger}(\mathbb{I})V(G)] u_{m0k_{\perp}}^{\dagger}} \left[\prod_{k_m}^{\pi \leftarrow 0} P \right]^{\dagger} \boxed{u_{p\pi k_{\perp}}^{\dagger} (V^{\dagger}(G)B(\mathbb{I})) u_{l-\pi k_{\perp}}}$$

$$= B_{0, k_{\perp}}^{nm \dagger}(\mathbb{I}) W_{\pi \leftarrow 0}^{mp \dagger}(k_{\perp}) B_{\pi, k_{\perp}}^{pl}(\mathbb{I})$$

$$W_{2\pi \leftarrow 0}(k_{\perp}) = W_{0 \leftarrow -\pi}(k_{\perp}) W_{\pi \leftarrow 0}(k_{\perp})$$

$$= B_{0, k_{\perp}}^{\dagger}(\mathbb{I}) [W_{\pi \leftarrow 0}^{\dagger}(k_{\perp})] B_{\pi, k_{\perp}}(\mathbb{I}) W_{\pi \leftarrow 0}(k_{\perp})$$

$$\det W_{2\pi \leftarrow 0}(k_{\perp}) = \det(B_{0, k_{\perp}}^{\dagger}(\mathbb{I})) \det(B_{\pi, k_{\perp}}(\mathbb{I}))$$

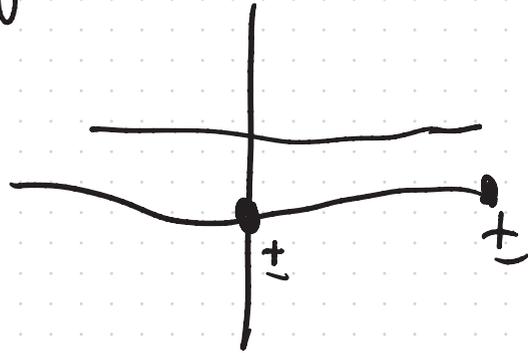
$$= \prod_{\text{occupied}} (\text{inversion eigenvalues @ } (0, k_{\perp})) (\text{inversion eigenvalues @ } (\pi, k_{\perp}))$$

s states

in particular, for a single band:

$$B_{0, k_{\perp}}^{(I)} = \pm 1$$

$$B_{\pi, k_{\perp}}^{(I)} = \pm 1$$



$$\det W = e^{i\varphi_B} = \begin{cases} 1 & \text{if } B_0 = B_{\pi} \rightarrow \varphi_B = 0 \\ -1 & \text{if } B_0 = -B_{\pi} \rightarrow \varphi_B = \pi \end{cases}$$