Lecture 21

Announcements:
- HW 5 will be posted nextweek 11/7
- Final presentations: ideas will be posted on course website.

Symmetries & the tight-binding Wilson loop

$$\tilde{P}_{ab}(\vec{k}) = \sum_{n=1}^{N_{occ}} u^{a}_{nk} \left(u^{b}_{nk}\right)^{*}$$ tight binding projection operator

$$W^{nm}_{k_\mu \leftarrow 0}(\vec{k}_\perp) = u^{\dagger}_{nk_\mu, k_\perp} \cdot \prod_{k_\mu'}^{k_\mu \leftarrow 0} \tilde{P}(k_\mu', k_\perp) \cdot \vec{u}_{m0, k_\perp}$$ - tight-binding Wilson line

On tight-binding basis functions: $g=\{\bar{g}|\vec{s}\}$ a symmetry

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

this is the "passive" perspective

Active: $U_g|\psi_{nk}\rangle\equiv|\psi'_{n\bar{g}k}\rangle$ $\qquad |\psi_{nk}\rangle=\sum_a u^a_{nk}|\chi_{ak}\rangle$

$$=\sum_a u^a_{nk}U_g|\chi_{ak}\rangle$$

$$=\sum_{ab}u^a_{nk}\quad B_{ba}(\bar{g})e^{-i\bar{g}k\cdot\vec{s}}|\chi_{b\bar{g}k}\rangle$$

define: $\boxed{\begin{aligned} u'_{n\bar{g}k} &= \sum_a e^{-i\bar{g}k\cdot\vec{\delta}} B_{ba}(\bar{g})\, u^a_{n\vec{k}} \\ |\psi'_{n\bar{g}k}\rangle &= \sum_a u'^{a}_{n\bar{g}k} |\chi_{a\bar{g}k}\rangle \end{aligned}}$

$B_{ab}(\bar{g})$ - $N\times N$ matrix

N - # of t.b. basis functions

$$\tilde{P}'_{ab}(\bar{g}k) = \sum_{n=1}^{N_{occ}} u'^{a}_{n\bar{g}k}\, u^{*\prime b}_{m\bar{g}k}$$

$$= \sum_{cd} B_{ac}(\bar{g})\, u^c_{nk}\, u^{*d}_{mk}\, B^\dagger_{db}(\bar{g})$$

$$= \left[B(\bar{g})\, \tilde{P}(k)\, B^\dagger(\bar{g}) \right]_{ab}$$

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

$$B^{nm}_{\vec{k}}(g) \equiv \vec{U}^\dagger_{n\bar{g}k} \cdot U'_{m\bar{g}k}$$

$$= u^\dagger_{n\bar{g}k} \cdot \left[B(\bar{g})\, e^{-i\bar{g}k\cdot\vec{\delta}} \right] u_{m\vec{k}}$$

Determine little grp representations for eigenstates

Inversion symmetry and the Wilson loop:

$g = \{I|\vec{0}\}$

$\bar{g} = I$

$\bar{g}k = -k$

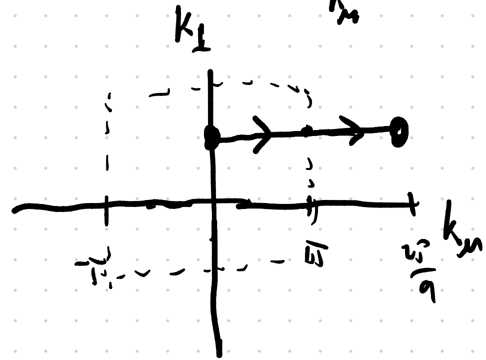
$$W^{nm}_{\frac{2\pi}{a}\leftarrow 0}(\vec{k}_\perp) = u^\dagger_{n\,\frac{2\pi}{a},k_\perp} \cdot \prod_{k_\mu'}^{\frac{2\pi}{a}\leftarrow 0} P(k_\mu', k_\perp)\, u_{m\,0,\vec{k}_\perp}$$

Periodicity of Bloch eigenvectors

$$u_{n\,\frac{2\pi}{a},\vec{k}_\perp} = V(\vec{b}_\mu)^\dagger u_{n\,0,k_\perp}$$

$$V_{ab}(\vec{b}_\mu) = e^{+i\vec{b}_\mu\cdot\langle r_a\rangle}\delta_{ab}$$

$$W^{nm}_{\frac{2\pi}{a}\leftarrow 0}(\vec{k}_\perp) = u^\dagger_{n,0,k_\perp} \cdot V(\vec{b}_\mu) \prod_{k_\mu'}^{\frac{2\pi}{a}\leftarrow 0} P(k_\mu', k_\perp)\, u_{m0,\vec{k}_\perp}$$



$$P(k_\mu' + \vec{b}_\mu, k_\perp)$$
$$= V^\dagger(b_\mu) P(k_\mu', k_\perp) V(b_\mu)$$

$$W^{nm}_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = u^\dagger_{n0k_\perp} V(b_\mu) \prod_{k_\mu'}^{\frac{2\pi}{a}\leftarrow\frac{\pi}{a}} P(k_\mu', k_\perp) \prod_{k_\mu''}^{\frac{\pi}{a}\leftarrow 0} P(k_\mu'', k_\perp)\, u_{m0,k_\perp}$$

$$= \left[u^\dagger_{n0k_\perp} \cancel{V(b_\mu)} \prod_{k_\mu'}^{0\leftarrow -\frac{\pi}{a}} \cancel{V^\dagger}(b_\mu) P(k_\mu', k_\perp) V(b)_\mu \prod_{k_\mu''}^{\frac{\pi}{a}\leftarrow 0} P(k_\mu'', k_\perp)\, u_{m0,k_\perp} \right]$$

$$\sum_{l=1}^{N_{occ}} u^{a}_{l\,\frac{\pi}{a},k_\perp} \, u^{b\dagger}_{l\,\frac{\pi}{a}\,k_\perp}$$

$$\boxed{W^{nm}_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = \sum_{l=1}^{N_{occ}} W^{nl}_{0\leftarrow -\frac{\pi}{a}}(k_\perp)\, W^{lm}_{\frac{\pi}{a}\leftarrow 0}(k_\perp)}$$

$$u_{l\,-\frac{\pi}{a},k_\perp} = V(b_n)\, u_{l,\frac{\pi}{a},k_\perp}$$

"Inversion-invariant momenta"

Let's let $\vec{k}_\perp$ be TRIM (time-reversal invariant momentum)

$\vec{k}_\perp = -\vec{k}_\perp + \vec{b}_\perp$ ~ $\vec{b}_\perp$ is a reciprocal lattice vector

$$\tilde{P}(k_n, k_\perp) = B^\dagger(I)\tilde{P}(-k_n, -k_\perp)B(I)$$

$$= B^\dagger(I)\tilde{P}(-k_n, k_\perp - \vec{b}_\perp)B(I)$$

$$= B^{+}(I)V(\vec{b}_\perp)\tilde{P}(-k_\mu, k_\perp)V^{+}(\vec{b}_\perp)B(I)$$

$$\prod_{k_\mu'}^{0\leftarrow -\frac{\pi}{a}} \tilde{P}(k_\mu, k_\perp) = \prod_{k_\mu''}^{0\leftarrow \frac{\pi}{a}} \tilde{P}(-k_\mu'', k_\perp)$$

$$= \prod_{k_\mu''}^{0\leftarrow \frac{\pi}{a}} \left[V^{+}(b_\perp)B(I)\tilde{P}(k_\mu, k_\perp)B^{+}(I)V(b_\perp)\right]$$

$$= V^{+}(b_\perp)B(I)\left[\prod_{k_\mu''}^{0\leftarrow \frac{\pi}{a}} \tilde{P}(k_\mu, k_\perp)\right]B^{+}(I)V(b_\perp)$$

$$= V^{+}(b_\perp)B(I)\left(\prod_{k_\mu''}^{\frac{\pi}{a}\leftarrow 0} \tilde{P}(k_\mu, k_\perp)\right)^{+}B^{+}(I)V(b_\perp)$$

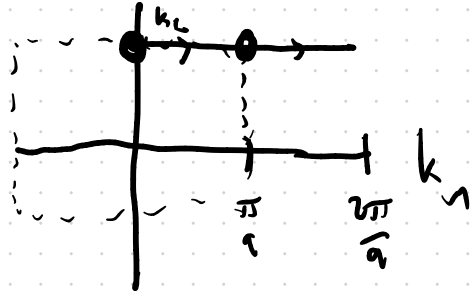
$$W^{nm}_{0\leftarrow -\frac{\pi}{a}}(k_\perp) = \left[u^\dagger_{n0k_\perp}\left[V^\dagger(b_1)B(I)\right]u_{l,0,k_\perp}\right]\left(W^{ll'}_{\frac{\pi}{a}\leftarrow 0}(k_\perp)\right)^\dagger\left[u^\dagger_{l',\frac{\pi}{a},k_\perp}B^\dagger V(b_1)u_{m\frac{\pi}{a}k_\perp}\right]$$

$$= B^{nl}_{0,k_\perp}(I)\left(W^{ll'}_{\frac{\pi}{a}\leftarrow 0}\right)^\dagger B^\dagger_{\frac{\pi}{a},k_\perp}(I)^{l'm}$$

This means for our Wilson loop

$$W_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = B_{0,k_\perp}(I)\left[W_{\frac{\pi}{a}\leftarrow 0}(k_\perp)\right]^\dagger B^\dagger_{\frac{\pi}{a},k_\perp}(I)\,W_{\frac{\pi}{a}\leftarrow 0}(k_\perp)$$

$$\det W_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = \left[\det B_{0,k_\perp}(I)\right]\left[\det B^\dagger_{\frac{\pi}{a},k_\perp}(I)\right]$$



$$= \prod_{\substack{\text{occupied} \\ \text{states}}} \left(\left(\text{inversion eigenvalues at } (0, k_\perp)\right)\left(\text{inversion eigenvalues at } \left(\tfrac{\pi}{a}, k_\perp\right)\right) \right)$$

One occupied band: $B_{0,k_\perp}(I) = \pm 1$

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

Berry phase

$$\det W = e^{i\varphi_B} = \begin{cases} +1 & \text{if } B_{0,k_\perp}(I) = B_{\frac{\pi}{a},k_\perp}(I) \rightarrow \varphi_B = 0 \\ -1 & \text{if } B_{0,k_\perp}(I) \neq B_{\pi/a,k_\perp}(I) \rightarrow \varphi_B = \pi \end{cases}$$

two dimensions:

$$h(k_x) = (\Delta + t_1 \cos k_x)\sigma_z + t_2 \sin k_x \sigma_y$$

$$|\Delta| > |t_1| \to \varphi_B = 0, \quad B^{--}_{k_x=0}(I) = B^{--}_{k_x=\frac{\pi}{a}}(I) = -1$$

$$|\Delta| < |t_1| \to \varphi_B = \pi \quad B^{--}_{k_x=0}(I) = -1, \quad B^{--}_{k_x=\frac{\pi}{a}}(I) = +1$$

$$h(k_x, k_y) = (\Delta + t_1 \cos k_x)\sigma_z + t_2 \sin k_x \sigma_y$$

$$+ \Delta \cos k_y \sigma_z + t_2 \sin k_y \sigma_x \leftarrow \text{Breaks time-reversal symmetry}$$

$$\sigma_z h(-k_x, -k_y)\sigma_z = h(k_x, k_y)$$

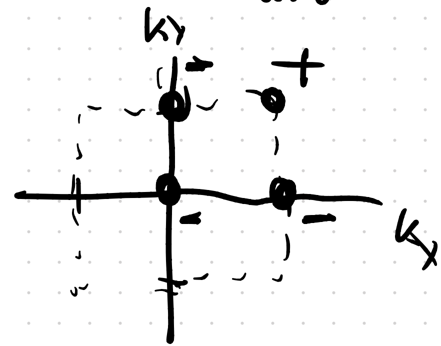
$$\varepsilon_\pm(k_x, k_y) = \pm\sqrt{(t_2 \sin k_y)^2 + (t_2 \sin k_x)^2 + (\Delta + t_1 \cos k_x + \Delta \cos k_y)^2}$$

$$\Delta > t_1 > 0$$
$$t_2 \neq 0$$

for 1×1 matrices ($\underline{1}$ occupied band)

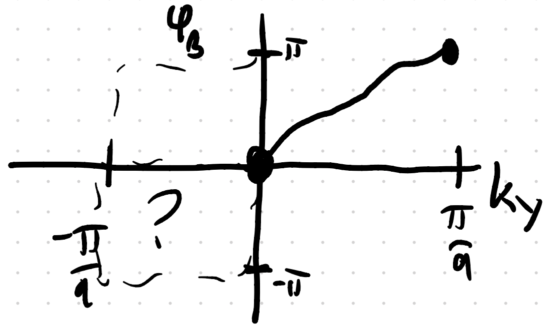
$$\det W = W$$

Inversion eigenvalues
for − band



$$W_{\frac{2\pi}{a}\leftarrow 0}(k_y) = \begin{cases} +1, & k_y = 0 \\ -1, & k_y = \frac{\pi}{a} \end{cases}$$

$$e^{i\varphi_B}$$



φ_B
π
$-\pi$
k_y
$\frac{\pi}{a}$
$-\frac{\pi}{a}$
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