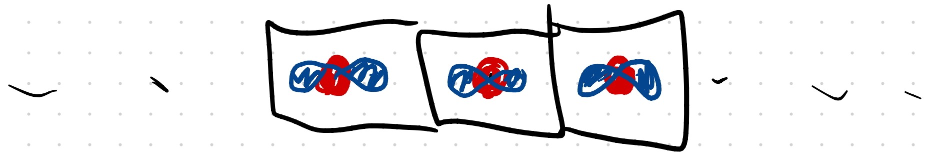
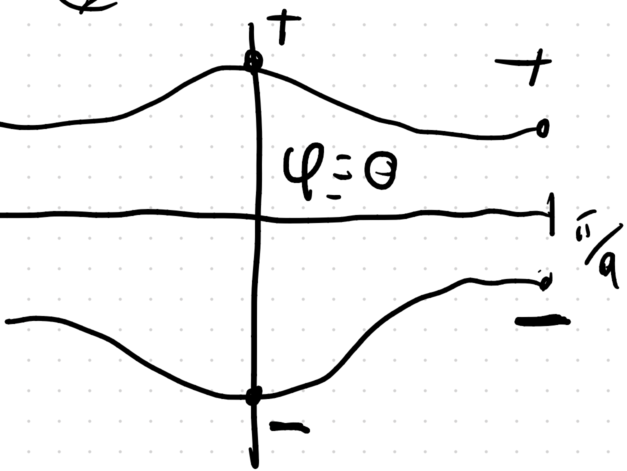
Lecture 21

Last time: 1d inversion-symmetric chain



Two distinct regimes

1



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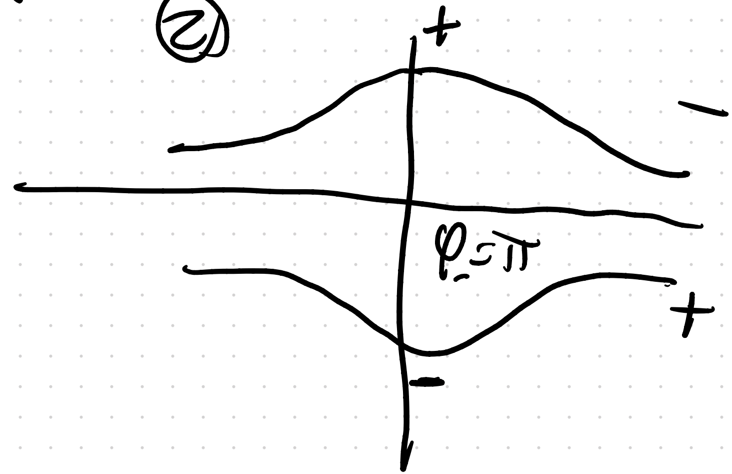
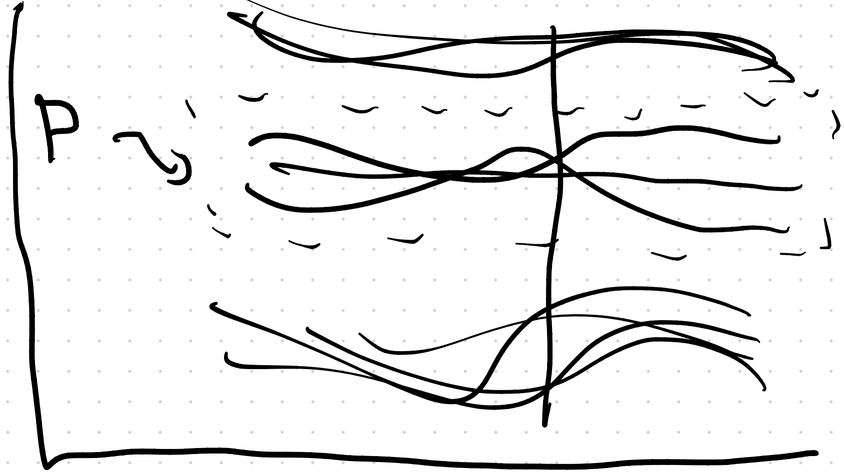


Inversion: $\varphi_- = 0, \text{ or } \pi \mod 2\pi$ quantized

Tight-binding basis

Projector onto occupied tb bands



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

$$= \frac{v}{(2\pi)^3} \int d^3k \sum_{n=1}^{N_{occ}} \sum_{ab} u_{nk}^{a} (u_{nk}^{b})^{*} |\chi_{ak}\rangle\langle\chi_{bk}|$$

define: $\tilde{P}_{ab}(k) = \sum_{n=1}^{N_{occ}} u_{nk}^{a} (u_{nk}^{b})^{*}$ matrix projects onto occupied $\vec{u}_{nk}$

→ Can rewrite the tight-binding Berry phase as a tight-binding wilson loop

$$W^{nm}_{\frac{2\pi}{a}\leftarrow 0}(\vec{k}_\perp) = \langle u_{n\,\frac{2\pi}{a},k_\perp} | \prod_{k_i}^{2\pi\leftarrow 0} P(k_i,k_\perp) | u_{m\,0,k_\perp} \rangle$$

$$\vec{u}^{\,\dagger}_{n,\frac{2\pi}{a},k_\perp} \cdot \prod_{k_i}^{\frac{2\pi}{a}\leftarrow 0} \tilde{P}_{ab}(k_i,k_\perp) \cdot u_{m0,k_\perp}$$

Tight-binding Wilson loop

$$P(k_i,k_\perp) = \sum_{n=1}^{N_{occ}} |u_{nk}\rangle\langle u_{nk}|$$

$$= \sum_{ab}^{N_{tot}} \sum_{n=1}^{N_{occ}} u^a_{nk} (u^b_{nk})^\dagger e^{-ikx} |\chi_{ak}\rangle\langle\chi_{bk}| e^{ikx}$$

$$= \sum_{ab}^{N_{tot}} \tilde{P}_{ab}(k) \, e^{-ikx} |\chi_{ak}\rangle\langle\chi_{bk}| e^{ikx}$$

Now: Suppose the tb basis fns form a band representation

$$g = \{\bar{g} | \vec{d}\} \in G$$

$$U_g |\chi_{ak}\rangle = \sum_{b=1}^{N_{tot}} |\chi_{b\,\bar{g}k}\rangle B_{ba}(\bar{g}) e^{-i\bar{g}k \cdot \vec{d}}$$

on eigenstates

$$U_g |\psi_{nk}\rangle \equiv |\psi'_{n\bar{g}k}\rangle$$ ← active transformation

$$= \sum_{a=1}^{N_{tot}} u^a_{nk}\, U_g |\chi_{ak}\rangle$$

in the 'tb limit, these do not contribute' to the Berry connection

N_{occ} = # of occupied bands

N_{tot} = # of bands in the model

$N_{tot} > N_{occ}$

$$= \sum_{a,b}^{N_{tot}} \underbrace{u^a_{nk} B_{ba}(\bar{g}) e^{-i\bar{g}k\cdot d}}_{u^{b\prime}_{n\bar{g}k} = \sum_{a=1}^{N_{tot}} B_{ba}(\bar{g}) e^{-i\bar{g}k} u^a_{nk}} |\chi_{b\bar{g}k}>$$

$$h_{ab}(k) u^b_{nk} = \varepsilon_{nk} u^a_{nk}, \quad B^\dagger(\bar{g}) h(\bar{g}k) B(\bar{g}) = h(k)$$

$$\Rightarrow \quad h_{ab}(\bar{g}k) u^{b\prime}_{n\bar{g}k} = \varepsilon_{nk} u^{b\prime}_{n\bar{g}k}$$

$\Rightarrow$ We can define the $N_{occ} \times N_{occ}$ Sewing matrix

$$\boxed{B^{nm}_{\vec{k}}(g) = \vec{u}^{\dagger}_{n\bar{g}k} \cdot \vec{u}'_{m\bar{g}k}}$$

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

$$= \vec{u}^{\dagger}_{n\bar{g}k} \cdot \Big[\underbrace{B(\bar{g})}_{\substack{N_{tot} \times N_{tot} \\ \text{matrix}}} e^{-i\bar{g}k \cdot \vec{d}} \Big] \vec{u}_{mk}$$

band representation

$$\boxed{\tilde{P}(\bar{g}k) = B(\bar{g}) \tilde{P}(k) B^{\dagger}(\bar{g})}$$

Lets focus on inversion symmetry

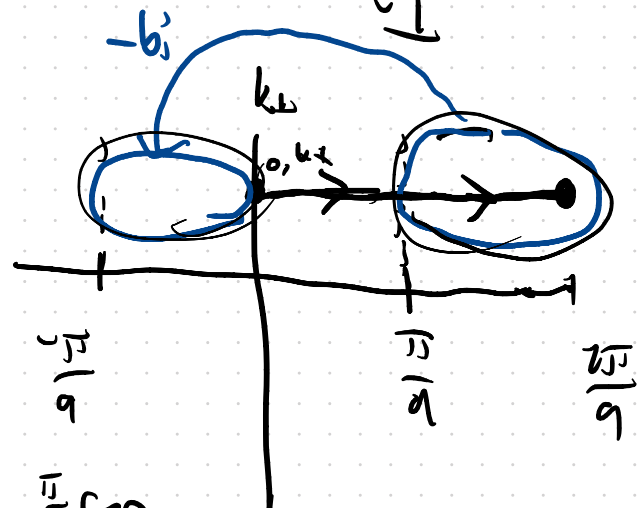
$$g = \{ I | 0 \} \qquad \bar{g} = I \qquad \bar{g}k = -k$$

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

Boundary conditions $\quad u_{n \frac{2\pi}{a}, k_\perp} = V^\dagger(\vec{b}_i) u_{n 0 k_\perp}$

$$= e^{-i b_i \cdot \vec{r}_a} \delta_{ab} u^b_{n 0 k_\perp}$$

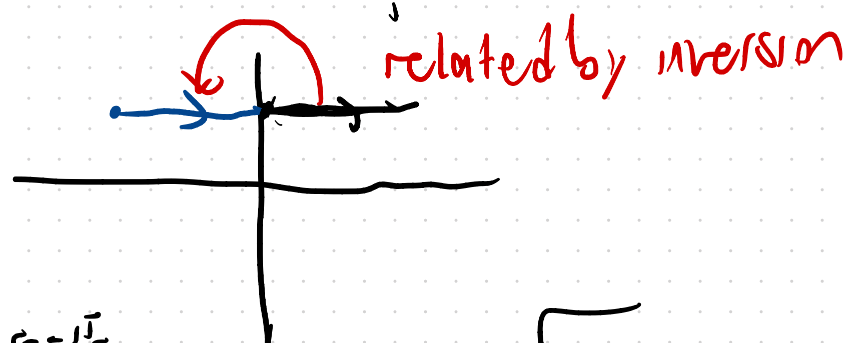
$$= \vec{u}^{\dagger}_{n0,k_\perp} \cdot V(b_i) \cdot \prod_{k_i}^{\frac{2\pi}{a} \leftarrow 0} \tilde{P}(k_i, k_\perp) \cdot \vec{u}_{n0k_\perp}$$



$$\prod_{k_i}^{\frac{2\pi}{a} \leftarrow 0} \tilde{P}(k_i, k_\perp) = \prod_{k_i}^{\frac{2\pi}{a} \leftarrow \frac{\pi}{a}} \tilde{P}(k_i, k_\perp) \prod_{k_i}^{\frac{\pi}{a} \leftarrow 0} \tilde{P}(k_i, k_\perp)$$

$$\tilde{P}(k_i, k_\perp) = V^{\dagger}(b_i)\, \tilde{P}(k_i - \vec{b}_i, k_\perp)\, V(b_i)$$

$$V^\dagger(b_j) \prod_{k_j}^{0\leftarrow -\frac{\pi}{a}} \tilde{P}(k_j,k_\perp) \Big) \, V(b_j) \prod_{k_j}^{\frac{\pi}{a}\leftarrow 0} \tilde{P}(k_j,k_\perp) \Big)$$



Holds regardless of symmetry

$$W^{mn}_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = \sum_{\ell=1}^{N_{occ}} \left[u^\dagger_{n,0,k_\perp} \prod_{k_j}^{0\leftarrow -\frac{\pi}{a}} \tilde{P}(k_j,k_\perp)\, u_{\ell,-\frac{\pi}{a},k_\perp}\right] \cdot \left[u^\dagger_{\ell,+\frac{\pi}{a},k_\perp} \prod_{k_j}^{\frac{\pi}{a}\leftarrow 0} \tilde{P}(k_j,k_\perp)\, u_{m,0,k_\perp}\right]$$

$$= \left[W_{0\leftarrow -\frac{\pi}{a}}(k_\perp) \cdot W_{\frac{\pi}{a}\leftarrow 0}(k_\perp)\right]^{nm}$$

Lets consider $k_\perp$ s.t. $-k_\perp = k_\perp - \vec{b}_\perp$

($k_\perp$ is a TRIM)

then $$\tilde{P}(k_i, k_\perp) = B^\dagger(I)\tilde{P}(-k_i, -k_\perp)B(I)$$
$$= B^\dagger(I)\tilde{P}(-k_i, k_\perp - b_\perp)B(I)$$
$$= B^\dagger(I)V(b_\perp)\tilde{P}(-k_i, k_\perp)V^\dagger(b_\perp)B(I)$$

Using this:

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

$$= \prod_{k_j}^{0\leftarrow -\frac{\pi}{a}} V^\dagger(b_\perp)B(I)\tilde{P}(k_j,k_\perp)B^\dagger(I)V(b_\perp)$$

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

$$W^{nm}_{0\leftarrow -\frac{\pi}{a}}(k_\perp) = \sum_l \tilde{u}_{n0k_\perp} V^\dagger(b_\perp)B(I)\tilde{u}_{l0k_\perp}\, u^\dagger_{l0k_\perp}\left(\prod_{k_j}^{\frac{\pi}{a}\leftarrow 0}\tilde{P}(k_j,k_\perp)\right)^\dagger$$

$$\times\sum_{l'} u_{l',\frac{\pi}{a},k_\perp}\, u^\dagger_{l',\frac{\pi}{a},k_\perp} B^\dagger(I)V(b_\perp)$$

$$= \rho^{ml}_{k=(0,k_\perp)}(I) \cdot \left[W^{\dagger}_{\frac{\pi}{a}\leftarrow 0}(k_\perp) \right]^{ll'} \rho^{l'n}_{k=(\frac{\pi}{a},k_\perp)}(I)$$

$\langle u_{m\,\frac{\pi}{a},k_\perp}$

$$\boxed{W_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = \rho_{k=(0,k_\perp)}(I)\, W^{\dagger}_{\frac{\pi}{a}\leftarrow 0}(k_\perp)\, \rho_{k=(\frac{\pi}{a},k_\perp)}(I)\, W_{\frac{\pi}{a}\leftarrow 0}(k_\perp)}$$

little group representation matrix for Inversion at k

$$\rho_k(I) = \vec{u}^{\dagger}_{n\,-k} \cdot B(I)\, u_{mk} \qquad k = -k + b_I$$

$$= u^{\dagger}_{nk} \cdot V^{\dagger}(b_I)\, B(I)\, u_{mk}$$

$$\det W_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = \det \rho_{(0,k_\perp)}(I) \det \rho_{(\frac{\pi}{a},k_\perp)}(I) \det \cancel{W_{\frac{\pi}{a}\leftarrow 0}}(k_\perp) \det \cancel{W^{\dagger}_{\frac{\pi}{a}\leftarrow 0}}(k_\perp)$$

$$e^{i\sum \varphi(k_\perp)}$$

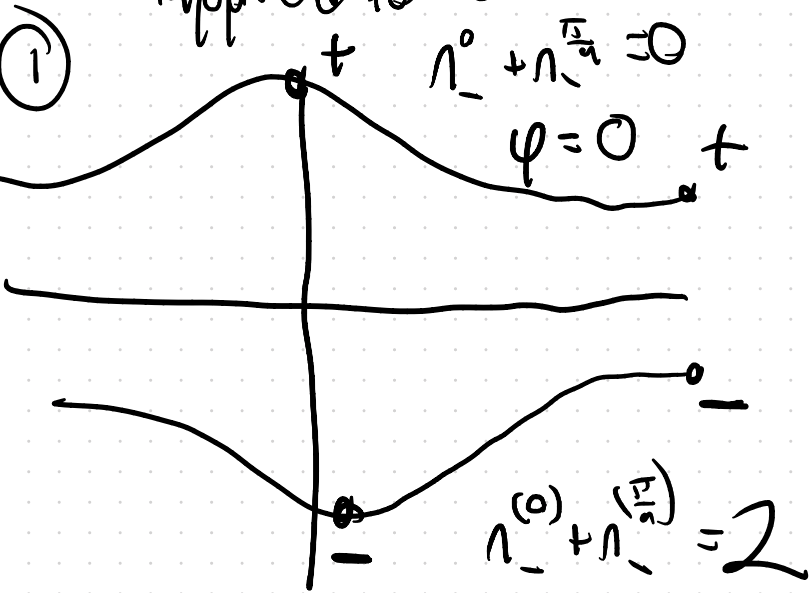
$$= \left(\prod_{\text{occupied states}} (\text{inversion eigenvalues at } (0,k_\perp))\right) \times \left(\prod_{\text{occupied states}} (\text{inversion eigenvalues at } (\tfrac{\pi}{a},k_\perp))\right)$$

$$\frac{2\pi}{ea} \cdot (p \bmod ea) = \pi \left(n_-^{(0,k_\perp)} + n_-^{(\frac{\pi}{a},k_\perp)} \right)$$

n_-^k - # of negative inversion eigenvalues at k

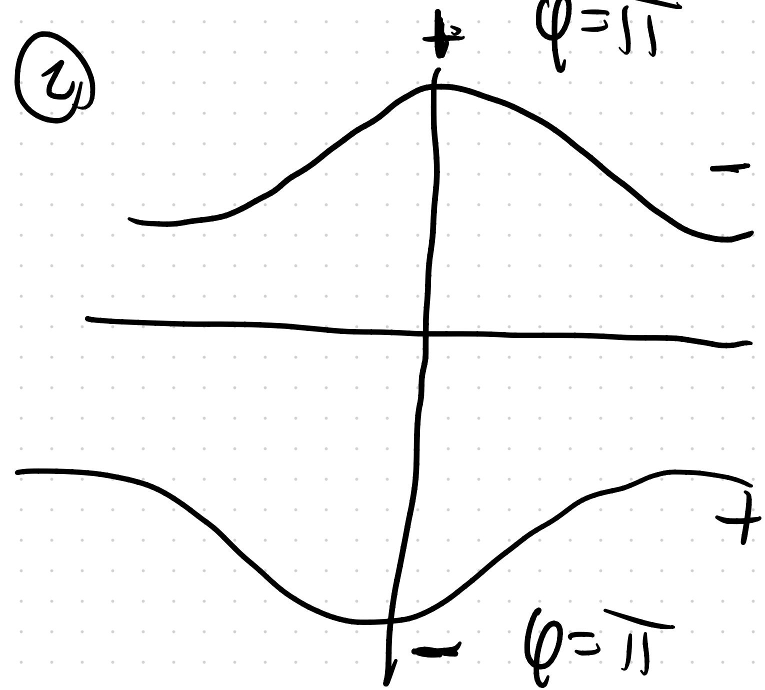
Applied to our 1d chain

1



$\varphi = 2\pi \bmod 2\pi = 0$

2



This is the first example of a symmetry indicator of band topology

[Berry phase invariant] $\longleftrightarrow$ [multiplicities of little grp representations]