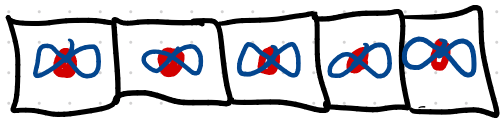
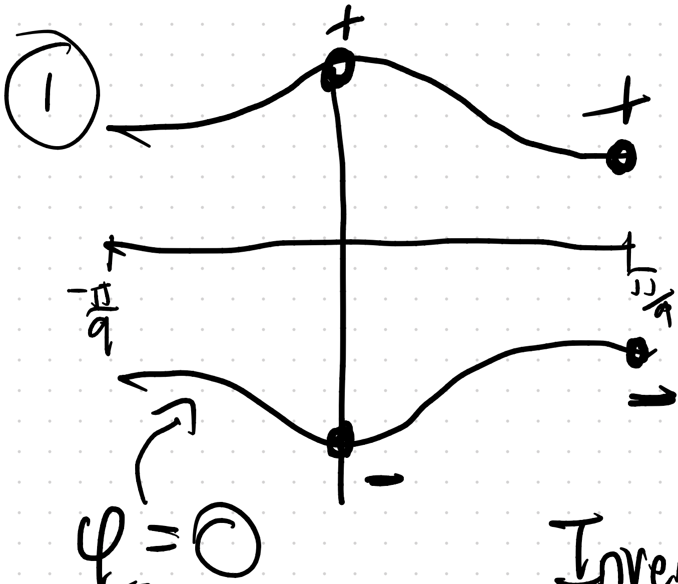
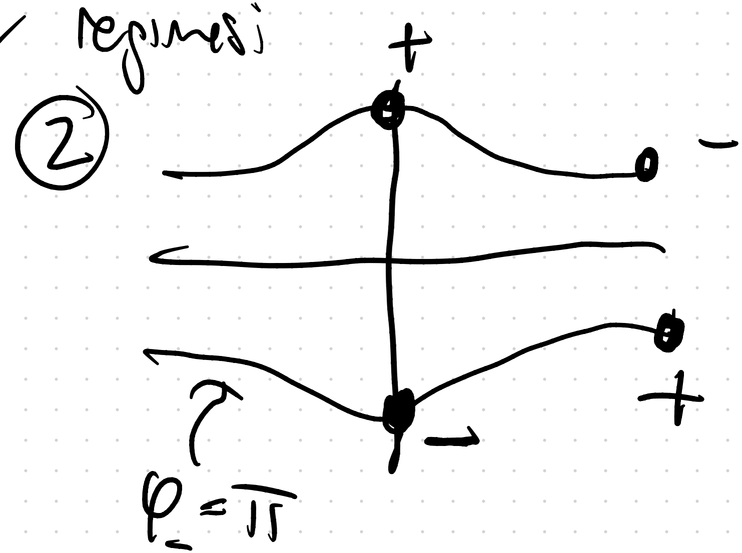
Lecture 21

Recap: 1D Inversion symmetric crystal

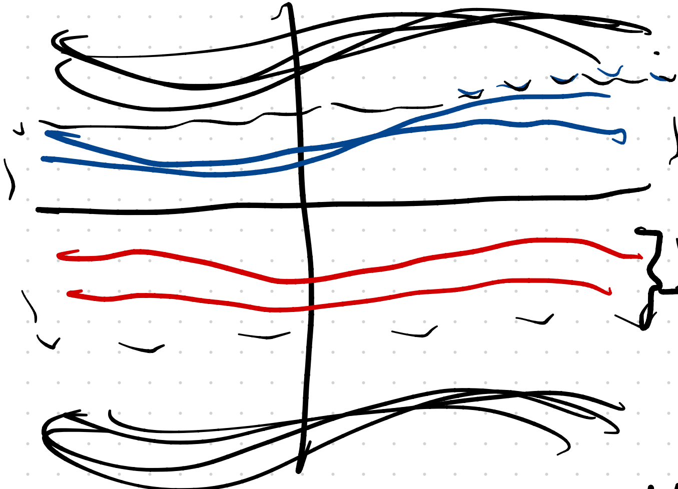


Two distinct insulating regimes:





Inversion: $\varphi_- = 0$ or π mod 2π
quantized



tight binding states $|\chi_{ak}\rangle, a=1,\dots N$

P onto N_{occ} states

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

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

define $\tilde{P}_{ab}(k) = \sum_{n=1}^{N_{occ}} (u^a_{nk}) (u^b_{nk})^*$

$$\sum_b \tilde{P}_{ab}(k)\, u^b_{mk} = \begin{cases} u^b_{mk} & \text{if } m \text{ is an occupied state} \\ 0 & \text{if } m \text{ is unoccupied} \end{cases}$$

$$P = \frac{V}{(2\pi)^3} \int d^3k \sum_{ab} |\chi_{ak}\rangle \tilde{P}_{ab}(k) \langle \chi_{bk}|$$

$$P(k) = \sum_{n=1}^{N_{occ}} |u_{nk}\rangle\langle u_{nk}| = \sum_{ab} e^{-ik\cdot x} |\chi_{ak}\rangle \tilde{P}_{ab}(k) \langle \chi_{bk}| e^{ik\cdot x}$$

We want to approximate Wilson loops

$$W^{nm}_{\frac{2\pi}{a}\leftarrow 0}(\vec{k}_\perp) = \langle u_{n,\frac{2\pi}{a},k_\perp}| \prod_{k_i}^{\frac{2\pi}{a}\leftarrow 0} P(k_i, k_\perp) |u_{m0,k_\perp}\rangle$$

$$P(k_i+\delta k, k_\perp)P(k_j, k_\perp)$$

$$\approx \left[P(k_i, k_\perp) + \delta k\, \partial_i P(k_i, k_\perp)\right] P(k_j, k_\perp)$$

in the tb limit

$$\boxed{W^{nn}_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) \approx \vec{u}^{\dagger}_{n,\frac{2\pi}{a},k_\perp} \cdot \prod_{k_i}^{\frac{2\pi}{a}\leftarrow 0} \tilde{P}(k_i, k_\perp) \cdot \vec{u}_{n0,k_\perp}}$$

Suppose our tb basis fns form a band representation

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

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

active perspective

$$\underline{u_g|\psi_{nk}\rangle} = |\psi'_{nk}\rangle = \sum_{a=1}^{N} u^{a}_{nk}\, u_g|\chi_{ak}\rangle$$

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

$$u^{b\,\prime}_{n\bar{g}k} = \sum_{a=1}^{N} B_{ba}(\bar{g}) e^{-i\bar{g}k\cdot\vec{d}}\, u^{a}_{nk}$$

Schrödiger Eqn:

$$\sum_{b=1}^{N} h_{ab}(k)\, u^{b}_{nk} = \varepsilon_{nk}\, u^{a}_{nk} \qquad B^{\dagger}(\bar{g})\, h(\bar{g}k)\, B(\bar{g}) = h(k)$$

$$\Rightarrow \sum_{b=1}^{N} h_{ab}(\bar{g}k)\, u^{b\,\prime}_{n\bar{g}k} = \varepsilon_{nk}\, u^{b\,\prime}_{n\bar{g}k} \qquad \tilde{P}(\bar{g}k) = B(\bar{g})\,\tilde{P}(k)\,B^{\dagger}(\bar{g})$$

We can define an $N_{occ} \times N_{occ}$ sewing matrix

$$\underbrace{B^{nm}_{\vec{k}}(g)}_{N_{occ}\times N_{occ}\text{ sewing matrix}} = \vec{u}^{\,\dagger}_{n\bar{g}k} \cdot \vec{u}^{\,\prime}_{m\bar{g}k} = \vec{u}^{\,\dagger}_{n\bar{g}k} \cdot \Big[\underbrace{B(\bar{g})}_{N\times N\text{ band representation matrix}} e^{-i\bar{g}k\cdot\vec{d}}\Big] \cdot \vec{u}_{mk}$$

Lets focus on Inversion symmetry $g = \{ I | \vec{0} \}$ $\bar{g} = I$

$\vec{d} = 0$

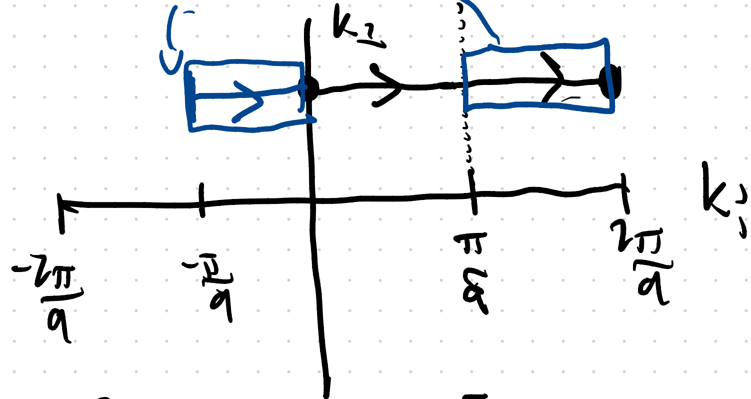
$$\bar{g} k = -k$$

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

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

$$= e^{-i \vec{b}_i \cdot \bar{r}_a} \delta_{ab} u^{b}_{n,0,k_\perp}$$

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



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

$$\tilde{P}(k_j,k_\perp) = V^\dagger(b_j)\,\tilde{P}(k_j-b_j,k_\perp)\,V(b_j)$$

$$= V^\dagger(b_j)\prod_{k_j}^{\frac{2\pi}{a}\leftarrow\frac{\pi}{a}} \tilde{P}\left(k_j-\frac{2\pi}{a},k_\perp\right)V(b_j)\prod_{k_j}^{\frac{\pi}{a}\leftarrow 0}\tilde{P}(k_j,k_\perp)$$

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

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

insert $\tilde{P}_{ab}\left(\frac{\pi}{a}, k_\perp\right) = \sum_{n=1}^{N_{occ}} u^a_{n \frac{\pi}{a}, k_\perp} u^{\dagger b}_{n \frac{\pi}{a}, k_\perp}$

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

Lets consider $k_\perp$ $\quad -k_\perp = k_\perp - \vec{b}_\perp$ ($k_\perp$ is a TRIM)

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

$$= B^\dagger(I)\,\tilde{\rho}(-k_j, k_\perp - b_\perp)\,B(I)$$

$$= B^\dagger(I)\,V(b_\perp)\,\tilde{\rho}(-k_j, k_\perp)\,V^\dagger(b_\perp)\,B(I)$$

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

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

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

$\tilde{\rho}$ hermitian $\rightarrow$

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

$$W^{nm}_{e\leftarrow -\frac{\pi}{a}}(k_1) = \sum_{l=1}^{N_{occ}} \left(\vec{u}^{\dagger}_{n0,k_1} \cdot V^{\dagger}(b_1) B(I) \vec{u}_{l0k_1}\right) u^{\dagger}_{l0k_1} \cdot \left(\prod_{k_i}^{\frac{\pi}{a}\leftarrow 0} P(k_i,k_1)\right)^{\dagger} \cdot \left(\sum_{l'=1}^{N_{oc}} u_{l',\frac{\pi}{a},k_1} \left(u^{\dagger}_{l',\frac{\pi}{a},k_1} \cdot B^{\dagger}(I) V(b_1) u_{m,-\frac{\pi}{a},k_1}\right)\right)$$

Sewing matrix for inversion @ $k=0,k_1$

Sewing matrix† at $k=(\frac{\pi}{a},k_1)$

$$= B_{k=(0,k_1)}(I) \cdot W^{\dagger}_{\frac{\pi}{a}\leftarrow 0}(k_1)\, B^{\dagger}_{k=(\frac{\pi}{a},k_1)}(I)$$

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

For $k_\perp$ a TRIM

since $\left(B_{k=(\frac{\pi}{a},k_\perp)}(I)\right)^2 = \mathrm{Id}$

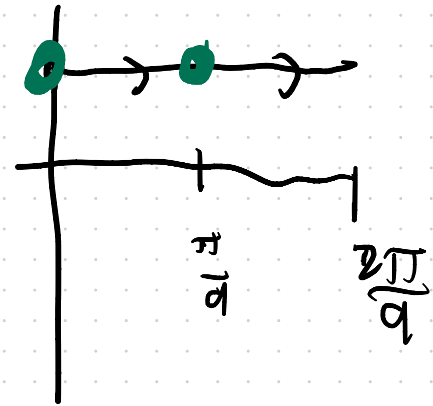
$$\boxed{W_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = B_{k=(0,k_\perp)}(I)\, W^\dagger_{\frac{\pi}{a}\leftarrow 0}(k_\perp)\, B_{k=(\frac{\pi}{a},k_\perp)}(I)\, W_{\frac{\pi}{a}\leftarrow 0}(k_\perp)}$$

little group representation matrices for inversion

$$\boxed{\det W_{\frac{2\pi}{a}\leftarrow 0}(k_\perp) = \det B_{k=(0,k_\perp)}(I)\, \det B_{k=(\frac{\pi}{a},k_\perp)}(I)} \times \cancelto{1}{\det W^\dagger_{\frac{\pi}{a}\leftarrow 0}(k_\perp) \det W_{\frac{\pi}{a}\leftarrow 0}(k_\perp)}$$

$$e^{i\sum_n \varphi_n(k_\perp)} = \left(\prod_{\substack{\text{occupied}\\ \text{state}}} \left(\text{inversion eigenvalues @ } (0,k_\perp)\right)\right)$$

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



polarization density

$$e^{\frac{2\pi i}{ea}(\vec{P})} = e^{i\pi n_-^{(0,k_\perp)}}\, e^{i\pi n_-^{(\frac{\pi}{a},k_\perp)}}$$

n_-^{k} = # of occupied negative inversion eigenvalues @ k

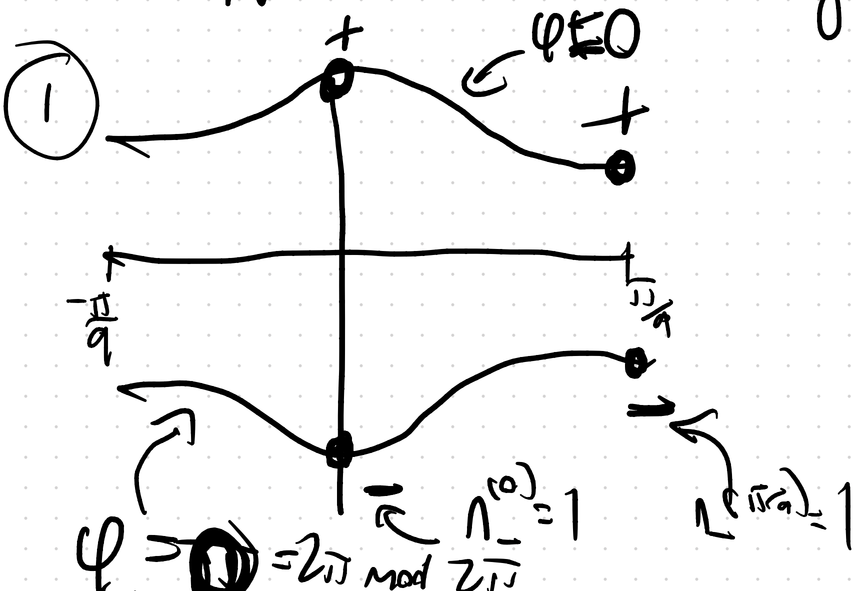
$$\boxed{\sum_n \varphi_n(k_\perp) \bmod 2\pi = \pi\left(n_-^{(0,k_\perp)} + n_-^{(\frac{\pi}{a},k_\perp)}\right)}$$

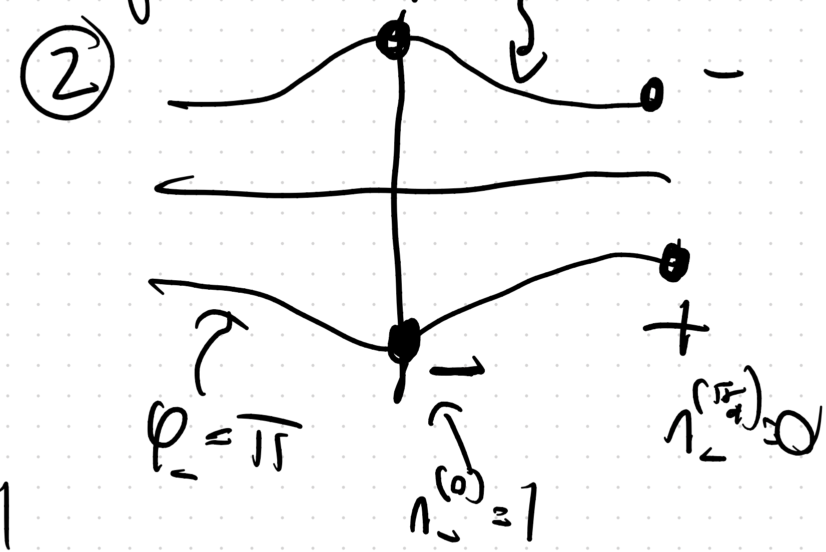
$$\boxed{\frac{2\pi}{ea}\left(\vec{p} \bmod ea\right)}$$

Apply to our 1D crystal

1 occupied band

Two distinct insulating regimes:





Symmetry indicator of band topology

[Berry phase invariant] $\longleftrightarrow$ [Multiplicities of little group reps in the occupied states]