Lecture 19

- Time-Reversal Symmetry: $T P_{x_1} P T^{-1} = P_{x_1} P$

  $W_{2\pi \leftarrow 0}(k_\perp)$ and $W_{2\pi \leftarrow 0}(-k_\perp)$ have the same spectrum

  If $T^2 = -1$ then Kramers' theorem

  $\Rightarrow$ Eigenvalues of $W_{2\pi \leftarrow 0}(k_\perp^*)$ are doubly degenerate $k_\perp^* \equiv -k_\perp^* \mod G$

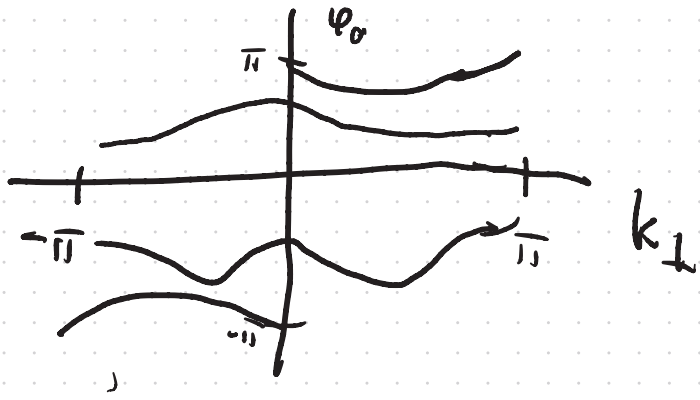
- Inversion symmetry $U_I P x_\mu P U_I^\dagger = -P x_\mu P$

$\Rightarrow$ $W_{2\pi\sigma=0}(k_\perp)$ and $W^*_{2\pi\sigma=0}(-k_\perp)$ have the same spectrum

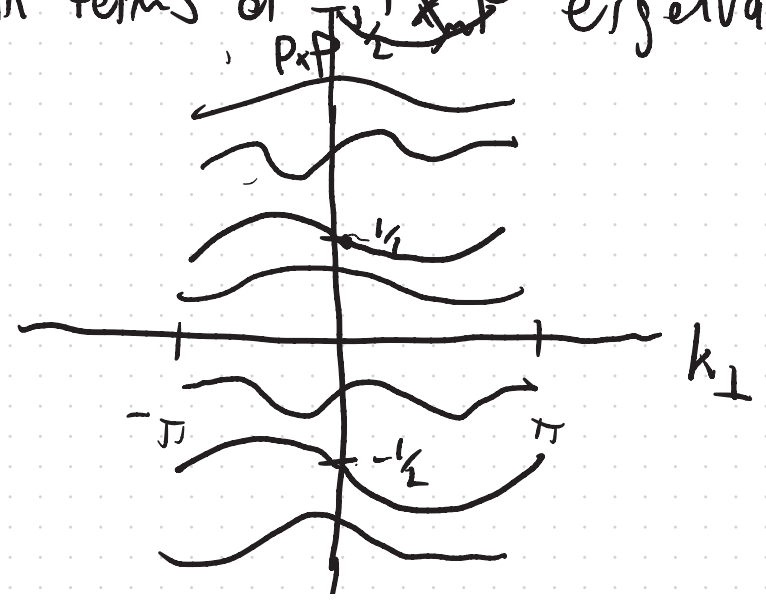
$$\{\varphi_a(k_\perp)\} = \{-\varphi_a(-k_\perp)\}$$

How do we plot Wilson loop eigenvalues:

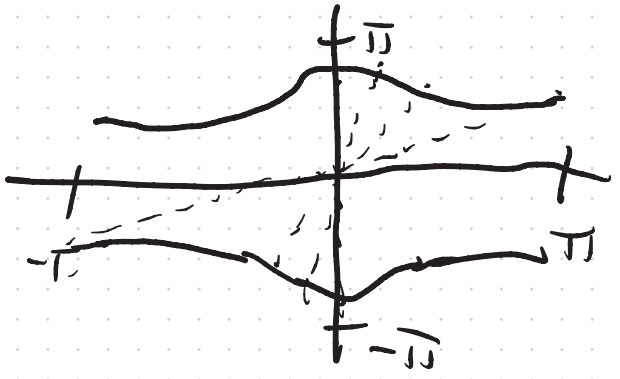
$$\lambda_a = e^{i\varphi_a(k_\perp)}$$



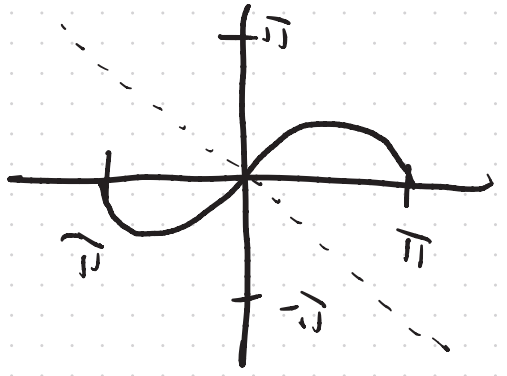
in terms of $P \times P$ eigenvalues $\left\{ z + \frac{\varphi_a(k_\perp)}{2\pi} \,\middle|\, z \in \mathbb{Z} \right\}$



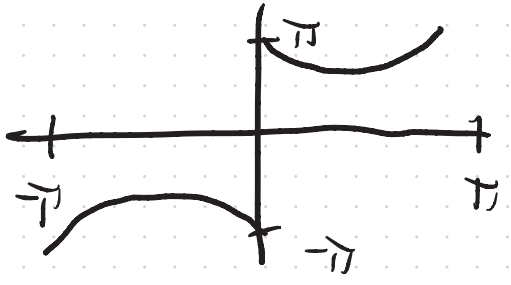
Inversion: $\{\varphi_a(k_\perp)\} = \{-\varphi_a(-k_\perp)\}$



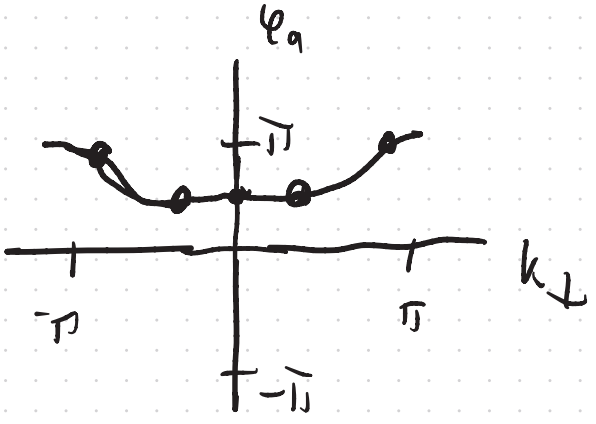
$k_\perp$



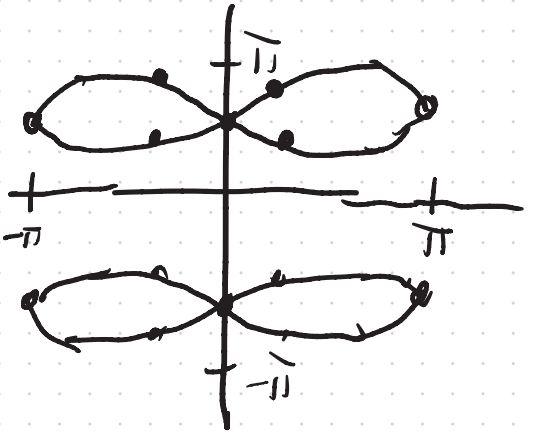
or



Time reversal symmetry $\{\varphi_a(k_\perp)\} = \{\varphi_a(-k_\perp)\}$



if $T^2 = +1$



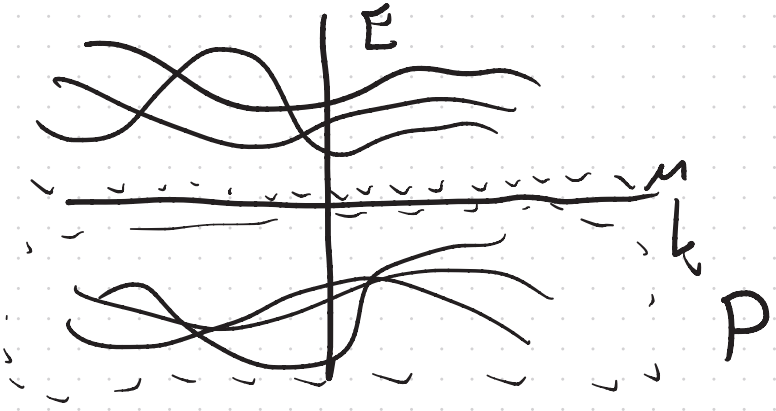
$T^2 = -1$

Connecting $P_{x_m}P$ eigenvalues to observables:

$$P x_\mu P |W_{az k_\perp}\rangle = \left(z + \frac{\varphi_a(k_\perp)}{2\pi}\right) |W_{az k_\perp}\rangle$$

$$\langle W_{az k_\perp} | x_\mu | W_{az k_\perp}\rangle = \left(z + \frac{\varphi_a(k_\perp)}{2\pi}\right)$$

$\frac{\varphi_a(k_\perp)}{2\pi}$ is the displacement of the center of charge of $|W_{az k_\perp}\rangle$ from the origin of the unit cell



P projects onto the occupied bands of this insulator w/ N occupied bands

$$\langle X_\mu \rangle = \frac{1}{(2\pi)^3} \int d^3k \sum_{n=1}^{N} \langle \psi_{nk} | X_\mu | \psi_{nk} \rangle$$

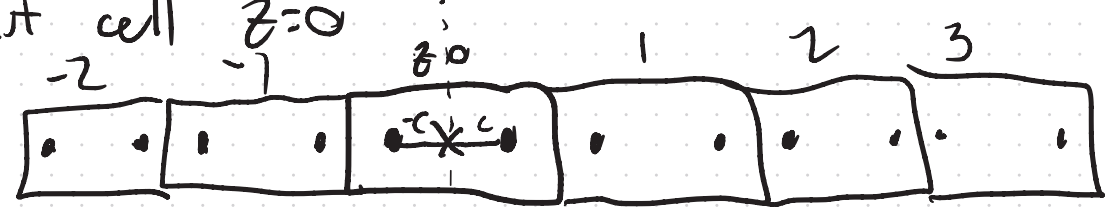
$$= \frac{1}{(2\pi)^2} \int d^2k_\perp \sum_{a=1}^{N} \sum_{z=-\infty}^{\infty} \langle W_{az k_\perp} | X_\mu | W_{az k_\perp} \rangle$$

$$= \frac{1}{(2\pi)^2} \int d^2k_\perp \sum_{q=1}^{N} \sum_{z=-\infty}^{\infty} \left(z + \frac{\varphi_q(k_\perp)}{2\pi} \right)$$

We can fix this by looking at the <u>dipole moment</u>

$$d_\mu = -e\langle x_\mu \rangle |a_\mu| + \sum_i Q^i_{ion} x^{ion}_\mu$$

We place the origin at the center of ionic charge in unit cell $z=0$



$$d_\mu = \underbrace{\cancel{\sum_{z=-\infty}^{\infty} N e \cancel{z}^{0} |a_\mu|}} - \frac{1}{(2\pi)^2} e|a_\mu| \sum_{a=1}^{N} \int d^2k_\perp \left(\cancel{z}^{0} \frac{\varphi_a(k_\perp)}{2\pi} \right)$$

$$d_\mu = \sum_{z=-\infty}^{\infty} \sum_{a=1}^{N} \int d^2k_\perp \frac{\varphi^a(k_\perp)}{(2\pi)^3} e|a_\mu|$$

$$= \sum_{z=-\infty}^{\infty} P_\mu$$

P_μ polarization density

dipole moment per unit cell

$$P_\mu = -e|a_\mu| \int d^2k_\perp \frac{1}{(2\pi)^3} \sum_{a=1}^{N} \varphi^a(k_\perp)$$

$$\sum_{a=1}^{N} \varphi^a(k_\perp) = \mathrm{Im} \log\left(e^{i\sum_{a=1}^{N} \varphi^a(k_\perp)}\right)$$

$$= \mathrm{Im} \log \prod_{a=1}^{N} e^{i\varphi^a(k_\perp)}$$

$$= \mathrm{Im} \log \det W$$

$$W = \mathcal{P} e^{i\int dk_\mu A_\mu(\vec{k})}$$

$$\det W = e^{i\int dk_\mu \, \mathrm{tr} A_\mu(\vec{k})}$$

$$(\log \det M = \mathrm{tr} \log M)$$

$$\sum_{a=1}^{N} \varphi^a(k_\perp) = \int \underline{dk_\mu}\, \mathrm{tr}(A_\mu(k_\mu, k_\perp))$$

$$\boxed{\rho_\mu = \frac{-e|a_\mu|}{(2\pi)^3} \int d^3k\, \mathrm{tr}\, A_\mu(k_\mu, k_\perp)}$$

What about gauge symmetry

$$A_\mu \to U^\dagger A_\mu U + i U^\dagger \partial_\mu U \qquad U = \begin{pmatrix} e^{i\theta_1} & & & \\ & e^{i\theta_2} & & \\ & & e^{i\theta_3} & \\ & & & \ddots \end{pmatrix}$$

$$\mathrm{tr}(A_\mu) \to \mathrm{tr}(U^\dagger A_\mu U) + i\, \mathrm{tr}(U^\dagger \partial_\mu U)$$

$$= \mathrm{tr}\, A_\mu + i\left(i\,\partial_\mu(\theta_1+\theta_2+\dots\theta_N)\right) \qquad \theta=\theta_1+\theta_2+\dots\theta_N$$

$$= \mathrm{tr}\, A_\mu - \partial_\mu\theta \qquad \text{if } U(\vec{k}) \text{ is periodic}$$

$$\theta(k_\mu+2\pi) = \theta(k_\mu)+2\pi m$$

$$\rho_\mu \to \rho_\mu + \frac{e|q_\mu|}{(2\pi)^3}\int d^3k\, \partial_\mu\theta$$

$$= \rho_\mu + e|q_\mu|\, m$$

$\to$ only the fractional part of $\rho_\mu / e|q_\mu|$ is gauge

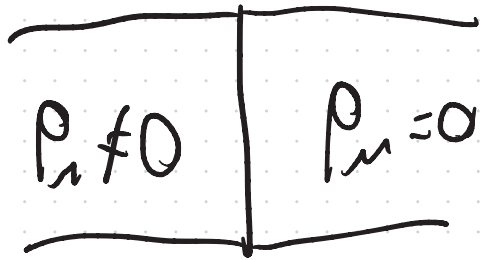
invariant

Maxwell eqns $\rho_b = -\nabla \cdot \frac{\vec{p}}{v}$

bound charge

dipole moment density

At boundaries



$\sigma_b = \rho_\mu / v$

Circling back: Can we get a set of Wannier functions that are well localized in <u>all</u> directions?

$$[x_\mu, x_\nu] = 0$$

if we want eigenstates of $Px_\mu P$ and $Px_\nu P$

we need $$[Px_\mu P, Px_\nu P] \overset{?}{=} 0$$

$$Px_\mu P x_\nu P - Px_\nu P x_\mu P$$

$$|f\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle f_{nk}$$

$$P x_\mu P |f\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle [i D_\mu f]_{nk}$$

$$[P x_\mu P, P x_\nu P]|f\rangle = \frac{-v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle \left(D_\mu D_\nu f - D_\nu D_\mu f\right)$$

$$D_\mu D_\nu f = (\partial_\mu - iA_\mu)(\partial_\nu - iA_\nu) f$$

$$= \partial_\mu \partial_\nu f - iA_\mu \partial_\nu f - i\partial_\mu (A_\nu f) - A_\mu A_\nu f$$

$$D_\nu D_\mu f = \partial_\nu \partial_\mu f - iA_\nu \partial_\mu f - i\partial_\nu (A_\mu f) - A_\nu A_\mu$$

$$\left(D_\mu D_\nu - D_\nu D_\mu\right) f = -i\left(\partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu]\right) f$$

$$= -i\, \Omega^{nm}_{\mu\nu} f_{mk}$$

$\boxed{\Omega_{\mu\nu} \text{ is the non-abelian Berry curvature}}$

$[P x_\mu P, P x_\nu P] = 0$ only if $\Omega_{\mu\nu}(\vec{k})$ vanishes for all $\vec{k}$

$$[P x_\mu P, P x_\nu P]|f\rangle = \frac{v}{(2\pi)^3}\int d^3k\, |\psi_{nk}\rangle\, i\Omega^{nm}_{\mu\nu}(k) f_{mk}$$