Lecture 23

- Final Presentations start in 2wks
- HW 5 posted, due 5/7 by 11:59pm

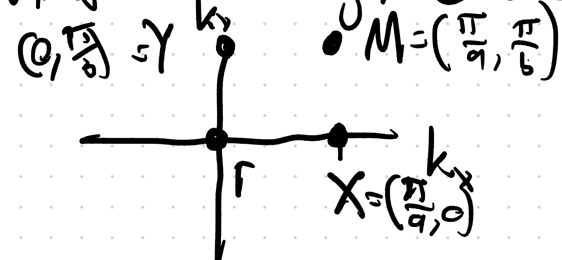
Recap: $$h(\vec{k}) = \left(\Delta[1+\cos k_y b] + t_1 \cos k_x a\right)\sigma_z + t_2 \sin k_x a\, \sigma_y - t_2 \sin k_y b\, \sigma_x$$ ← Breaks TRS, preserves I

$B(I) = \sigma_z$

($\Delta, t_1 > 0$)

Inversion eigenvalues for negative energy band

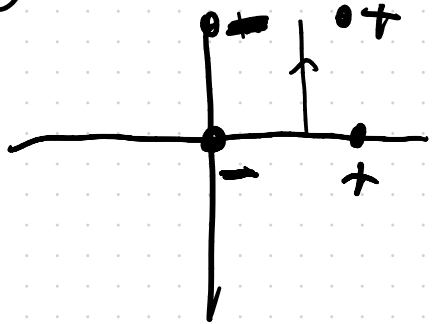
h

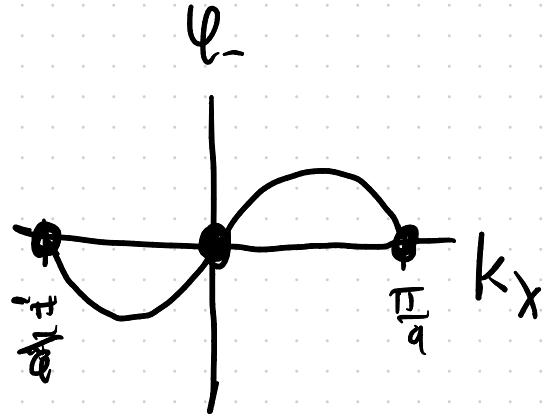


$$e^{i\varphi_-} = (-1)^{n_-}$$

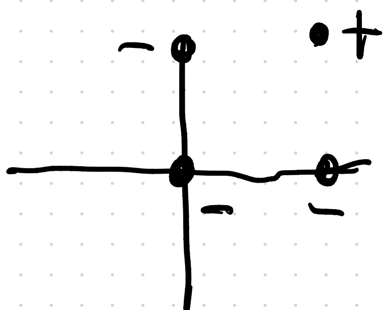
Two phases

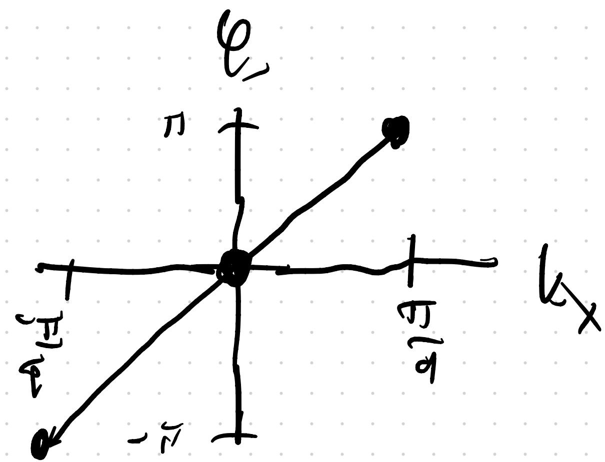
① $t_1 > 2\Delta > 0$





② $2\Delta > t_1 > 0$



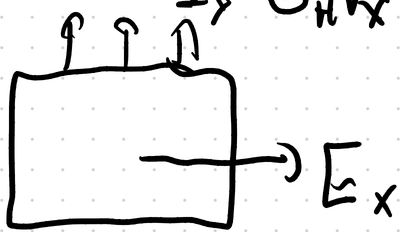


Chern number $C = \frac{1}{2\pi} \int dk_x \frac{\partial}{\partial k_x} \operatorname{Im} \log \det W_{\frac{2\pi}{b} \leftarrow 0}(k_x)$

$$= \frac{1}{2\pi} \oiint d^2k \, \operatorname{tr} \underbrace{\Omega_{xy}}_{\text{Berry curvature}}$$

① $C \in \mathbb{Z}$ - C can't change under perturbations if a gap remains open - topological invariant

$I_y = G_H V_x$

② 

$G_H = C \, q^2/h$ Hall conductance

③ If we have inversion symmetry

Symmetry indicator formula $\rightarrow$ $$(-1)^C = \prod_{\substack{k_* \in \text{TRIM} \\ \text{no occ}}} \xi_n(k_*)$$ $\pm 1 = \xi_n(k_*)$ are the inversion eigenvalues

Note: C can be defined and is invariant regardless of whether we have inversion symmetry

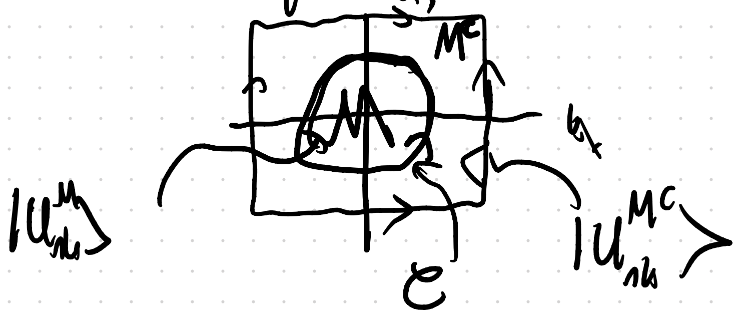
④ Claim: $C \neq 0 \rightarrow$ the occupied bands do not have exponentially localized Wannier functions

$$|W_{\vec{R}}\rangle = \frac{V}{(2\pi)^3} \int d^3k \, |\psi_k\rangle U(k) e^{-ik\cdot R}$$

Try to choose $U(k)$ s.t. $|\tilde{\psi}_k\rangle = |\psi_k\rangle U(k)$ is a smooth function of $\vec{k}$

Sketch of proof

occupied Bloch states
$|u^M_{nk}\rangle, |u^{M^c}_{nk}\rangle$



$\mathrm{tr}\,\Omega = \nabla \times \mathrm{tr}\,A$

$$C = \frac{1}{2\pi} \oint d^3k \ \mathrm{tr}\,\Omega = \frac{1}{2\pi}\left[\iint_M d^2k \ \mathrm{tr}\,\Omega + \iint_{M^c} d^2k \ \mathrm{tr}\,\Omega\right]$$

$$= \frac{1}{2\pi}\left[\oint_{\mathcal{C}} dk \cdot A_M - \oint_{\mathcal{C}} dk \cdot A_{M^c}\right]$$

$$A_M = i\langle u^M_{nk} | \nabla_k u^M_{mk}\rangle \qquad A_{M^c} = i\langle u^{M^c}_{nk} | \nabla_k u^{M^c}_{mk}\rangle$$

On $\mathcal{C}$, $\nabla \times \mathrm{tr} A_M = \nabla \times \mathrm{tr} A_{M^c}$

$$\Rightarrow \mathrm{tr} A_{M^c} = \mathrm{tr} A_M - \nabla \varphi$$

$$C = \frac{1}{2\pi} \oint_{\mathcal{C}} \nabla \varphi \cdot d\vec{k} \qquad |u^{M^c}_{nk}\rangle = e^{i\varphi(k)} |u^M_{nk}\rangle$$

$C \neq 0$ φ winds as we go around $\mathcal{C}$

$\Rightarrow$ φ is singular somewhere in the BZ

→ there is no single smooth gauge for our Bloch functions → No exponentially localised Wannier Functions

Now - Time-reversal Symmetry

$TRS \Rightarrow C=0$

Time-reversal symmetry T antiunitary

$$\langle v|w\rangle = \langle Tw|Tv\rangle$$

$$T P(k) T^{-1} = P(-k)$$

$$W_{\frac{2\pi}{b}\leftarrow 0}(k_x) = \left[\langle u_{n k_x, \frac{2\pi}{b}} | \prod_{k_y}^{\frac{2\pi}{b}\leftarrow 0} P(k_x, k_y)\right]\left[| u_{m k_x, 0}\rangle\right]$$

$$\langle v | w \rangle$$

$$|v\rangle = \prod_{k_y}^{0\leftarrow\frac{2\pi}{b}} P(k_x, k_y) | u_{n k_x, \frac{2\pi}{b}}\rangle$$

$$|w\rangle = |u_{m k_x, 0}\rangle$$

$$= \langle T u_{m k_x, 0} | T \prod_{k_y}^{0\leftarrow\frac{2\pi}{b}} P(k_x, k_y) | u_{n k_x, \frac{2\pi}{b}}\rangle$$

Sewing matrix: $B_k^{nm}(T) = \langle u_{n-k} | T u_{mk}\rangle$

$$= \sum_{ll'} B^{ml'\dagger}_{k_x,0}(T) \langle u_{l', -k_x, 0} | \prod_{k_y}^{0 \leftarrow 2\pi/b} P(-k_x, -k_y) | u_{l, -k_x, -\frac{2\pi}{b}} \rangle B^{l'n}_{k_x, \frac{2\pi}{b}}(T)$$

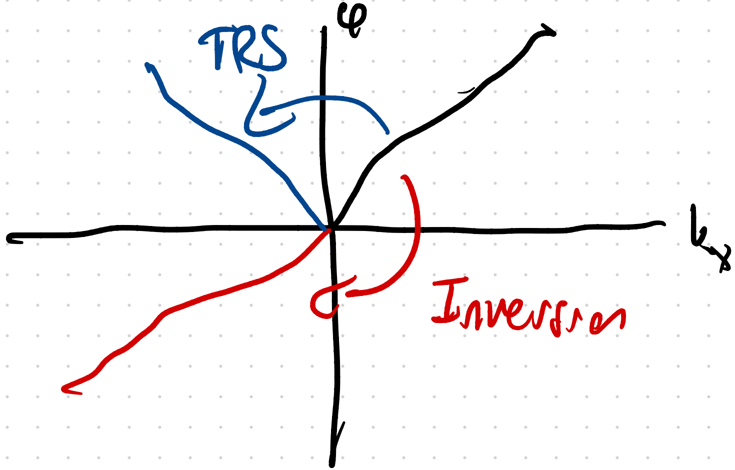
$$= B^\dagger(T) W^T_{\frac{2\pi}{b} \leftarrow 0}(-k_x) B(T) = W_{\frac{2\pi}{b} \leftarrow 0}(k_x)$$

has eigenvalues $e^{i\gamma_a(k_x)}$

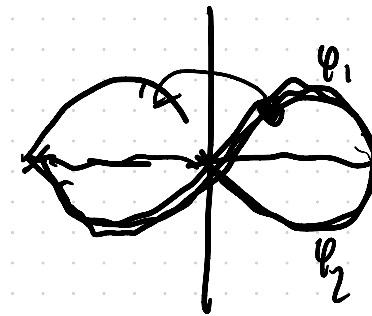
Has eigenvalues $e^{i\gamma_a(k_x)}$

$\Rightarrow W_{\frac{2\pi}{b} \leftarrow 0}(-k_x)$ has the same eigenvalues as $W_{\frac{2\pi}{b} \leftarrow 0}(k_x)$

$$\{\gamma_a(k_x)\} = \{\gamma_a(-k_x)\}$$



TRS: Wilson loop spectrum is symmetric under $k_x \leftrightarrow -k_x$



TRS: $\det W(k_x) = \det W(-k_x)$

$$C = \frac{1}{2\pi} \int_{-\pi/a}^{\pi/a} dk_x \frac{\partial}{\partial k_x} \operatorname{Im} \log \det W(k_x)$$

$$= \frac{1}{2\pi} \left[\int_{-\frac{\pi}{a}}^{0} dk_x \frac{\partial}{\partial k_x} \operatorname{Im} \log \det W(k_x) + \int_{0}^{\pi/a} dk_x \operatorname{Im} \log \det W(k_x) \right]$$

$$= \frac{1}{2\pi}\left[\int_0^{\sqrt{3}/a} dk_x \frac{\partial}{\partial k_x} \mathrm{Im} \log\det W - \frac{\partial}{\partial k_x} \mathrm{Im} \log\det W\right] = 0$$

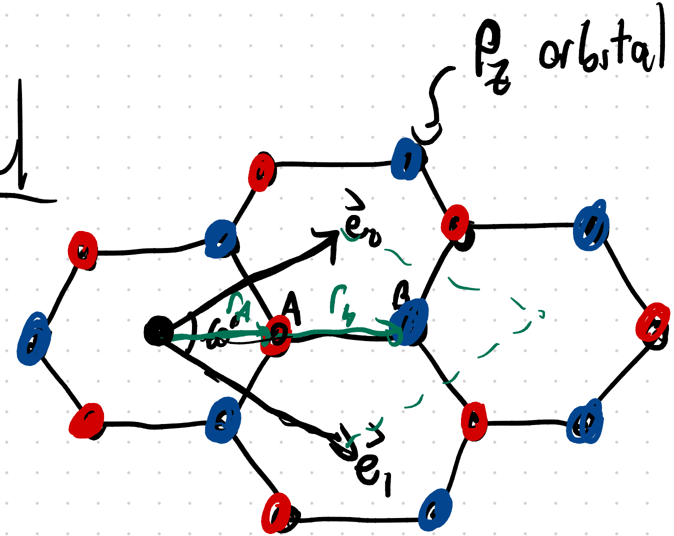
Kane Mele Model

$$\vec{e}_1 = \frac{a}{2}(\sqrt{3}\hat{x} - \hat{y})$$

$$\vec{e}_2 = \frac{a}{2}(\sqrt{3}\hat{x} + \hat{y})$$

$$\vec{r}_A = \frac{1}{3}\vec{e}_1 + \frac{1}{3}\vec{e}_2$$

$$\vec{r}_B = \frac{2}{3}\vec{e}_1 + \frac{2}{3}\vec{e}_2$$



two orbitals per unit cell

Pt group Symmetries

C_{6z}: 60° rotation about z axis

$$C_{6z}\vec{e}_1 = \vec{e}_2$$

$$C_{6z}\vec{e}_2 = \vec{e}_2 - \vec{e}_1$$

$$C_6\vec{r}_A = \frac{1}{3}\left(C_6\vec{e}_1 + C_6\vec{e}_2\right)$$

$$= \frac{1}{3}\left(\vec{e}_2 + \vec{e}_2 - \vec{e}_1\right)$$

$$= \frac{2}{3}\vec{e}_2 - \frac{1}{3}\vec{e}_1 = r_B - \vec{e}_1$$

$$C_6\vec{r}_B = \vec{r}_A - \vec{e}_1 + e_2$$

+ TRS

+ Inversion

I: $(x, y, z=0) \to (-x, -y, z=0)$

+ $M_y = M_{1\bar{1}}$: $\vec{e}_1 \leftrightarrow \vec{e}_2$

$\begin{matrix} 1 & \bar{1} \\ \uparrow & \uparrow \\ e_1 & -e_2 \end{matrix}$

$\vec{r}_A \to \vec{r}_A$

$\vec{r}_B \to \vec{r}_B$

Space group $P6/mmm1'$

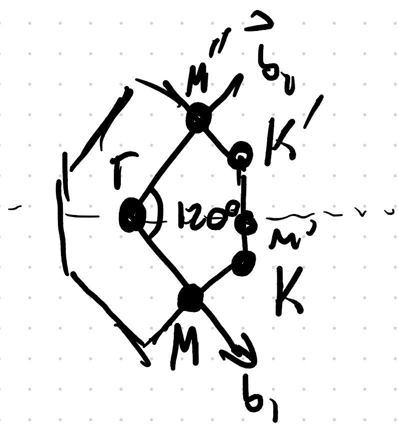
primitive (hexagonal) → P

C_{6z} → 6

Inversion → $/$

$M_{1\bar{1}}, M_{01}, M_z$ → mmm

Reciprocal lattice / BZ



$$\vec b_1 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{x} - \hat{y}\right)$$

$$\vec b_2 = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{x} + \hat{y}\right)$$

$$\text{TRIM}\begin{cases} \Gamma = \vec{0} \\ M = \frac{1}{2}\vec b_1 \quad M' = \frac{1}{2}\vec b_2 \quad M'' = \frac{1}{2}(\vec b_1 + \vec b_2) \end{cases}$$

$$K = \frac{2}{3}\vec b_1 + \frac{1}{3}\vec b_2$$

$$\vec{K} = \frac{2}{3}\vec{b}_2 + \frac{1}{3}\vec{b}_1$$

Little groups:

$$G_\Gamma = p6/mmm1'$$

$$G_M = pmmm1'$$

$$G_K \ni C_{3z},\ C_{6z}M_y = M_{01} = p3m$$