

Lecture 23

- HW 5 posted
- Solutions for HW 3 posted
- HW 3 graded

Reminder: Email me your presentation topics

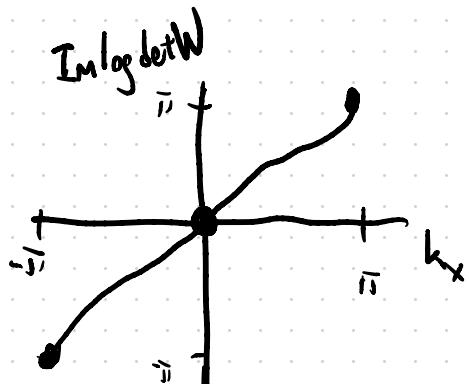
Chem insulator (with inversion symmetry)

$$\vec{h}(k) = (\Delta + \Delta \cos k_y + t_1 \cos k_x) \sigma_z + t_2 \sin k_x \sigma_y + t_2 \sin k_y \sigma_x$$

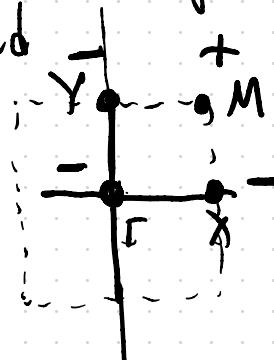
$$B(I) = \sigma_z$$

Two phases

$$\textcircled{1} \quad |2\Delta| > t_1, \quad \Delta, t_1, t_2 > 0$$



Inversion eigenvalues for occupied band



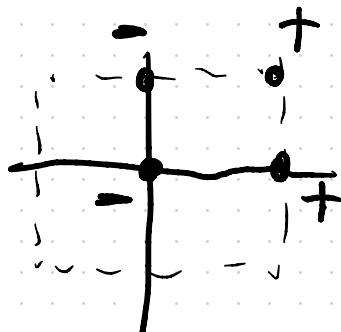
Chern number

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

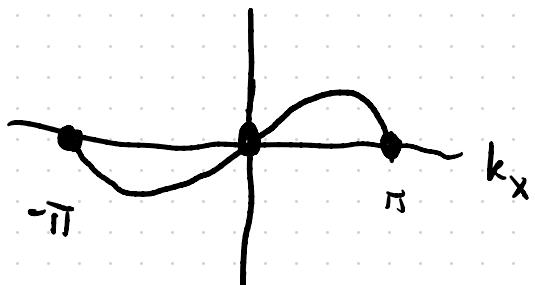
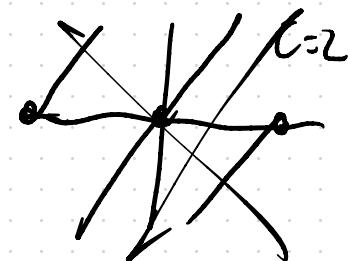
$$= \frac{1}{2\pi} \oint_{BZ} d^2k \text{tr}(\Omega) \quad \text{Berry curvature}$$

$\epsilon \not\in$ $C=1$

$$\textcircled{2} \quad 2\Delta < t_1, \Delta, t_1 > 0$$



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

 $\text{In } 1/\omega \text{ dt/dW}$  $C=0$ 

$$(-1)^C = \prod_{\substack{\text{Inversion} \\ \text{invariant Momentum} \\ k_x}} B_{k_x}^{-}(I) \leftarrow \begin{matrix} \text{Symmetry} \\ \text{Indicator formula} \end{matrix}$$

CFO: Nonzero Hall conductivity

- No exponentially localized Wannier functions - occupied band is topologically nontrivial

$$\det W(k_1) = e^{i\gamma(k_1)}$$

$$\det W(k_1 + \vec{b}_1) = \det W(k_1)$$

$$\gamma(k_1 + \vec{b}_1) = \gamma(k_1) + 2\pi C$$

Now: Time-reversal symmetry: Time-reversal symmetry
 $\Rightarrow C = 0$

$$W_{2\pi \leftarrow 0}^{nm}(k_x) = \langle u_{n k_x, 2\pi} | \prod_{k'_y}^{2\pi \leftarrow 0} P(k_x, k'_y) | u_{m k_x, 0} \rangle$$

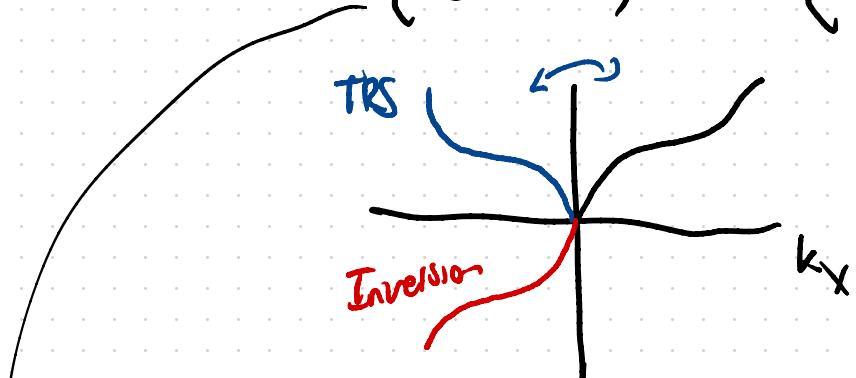
$$B(T) W_{2\pi \leftarrow 0}(k_x) B^{-1}(T) = W_{2\pi \leftarrow 0}^+(-k_x)$$

Since T is represented by an antiunitary operator:

$$\text{if } W_{2\pi \leftarrow 0}(k_x) |W_{k_x}\rangle = e^{i\gamma(k_x)} |W_{k_x}\rangle$$

$$W_{2\pi \leftarrow 0}^+(k_x) U_T |W_{k_x}\rangle = e^{-i\gamma(k_x)} U_T |W_{k_x}\rangle$$

Eigenvalues $\{e^{i\gamma_i(k_x)}\} = \{e^{i\gamma_i(-k_x)}\}$



$$\det W(k_x) = \det W(-k_x) = e^{i\gamma(k_x)}$$

$$C = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x \frac{\partial}{\partial k_x} \gamma(k_x) = \frac{1}{2\pi} \int_{-\pi}^0 dk_x \frac{\partial \gamma}{\partial k_x} + \int_0^{\pi} dk_x \frac{\partial \gamma}{\partial k_x} = 0$$

Kane-Mele model:

Space group

Primitive hexagonal

P6/mmm

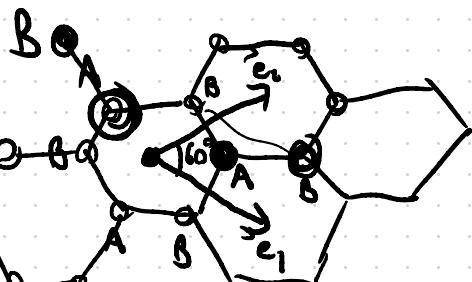
5-fold
rotation

$\begin{smallmatrix} & & 1 \\ & & \swarrow \text{time reversal} \end{smallmatrix}$

Mirror symmetry

Inversion
symmetry

$\begin{smallmatrix} 1 \\ \text{time-reversal} \\ \text{symmetry} \end{smallmatrix}$



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

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

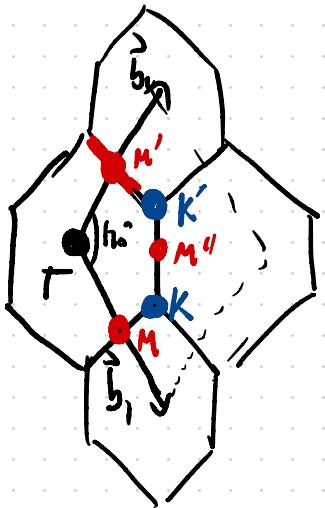
$$\vec{b}_1 = \frac{2\pi}{a} \left(\frac{\vec{x}}{\sqrt{3}} - \vec{y} \right)$$

Primitive Bravais lattice vectors

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

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

$$\vec{b}_0 = \frac{2\pi i}{a} \left(\frac{x}{\sqrt{3}} + \vec{y} \right)$$



$$\Gamma = 0$$

$$M = \frac{1}{2} \vec{b}_1$$

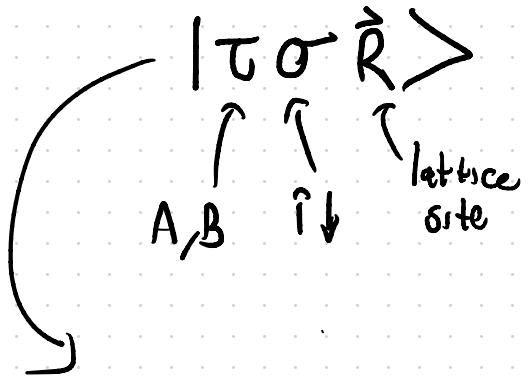
$$M'' = \frac{1}{2} \vec{b}_1 + \frac{1}{2} \vec{b}_2$$

$$M' = \frac{1}{2} \vec{b}_2$$

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

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

tight binding basis functions



3fold rotation symmetry

$$U_{C_3} |A\sigma\rangle = e^{\frac{-i\pi\sigma_z}{3}} |A\sigma - \vec{e}_1\rangle$$

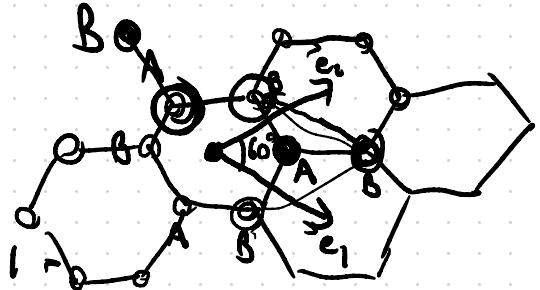
$$U_{C_3} |B\sigma\rangle = e^{\frac{-i\pi\sigma_z}{3}} |B\sigma - 2\vec{e}_1\rangle$$

Inversion: $U_I |A\sigma\rangle = |B\sigma - \vec{e}_1 - \vec{e}_2\rangle$

$$U_I |B\sigma\rangle = |A\sigma - 2\vec{e}_1 - \vec{e}_2\rangle$$

Fourier space

$$\boxed{B(I) = T_X \sigma_0}$$



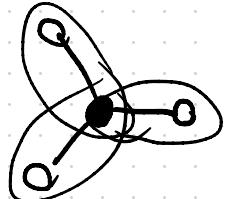
$$B(C_3) = T_0 e^{-i\pi \sigma_2 / 3}$$

$$B(C_2) = T_0 e^{-i\pi \sigma_3}$$

Nearest Neighbor spin independent tight binding model

$$h(R-R') = \langle \tau \sigma \vec{R} | H | \tau' \sigma' \vec{R}' \rangle$$

Nearest neighbors of $|A\sigma\rangle$ are



$$\left\{ \begin{array}{l} |B\sigma \vec{0}\rangle \\ |B\sigma -\vec{e}_1\rangle \\ |B\sigma -\vec{e}_2\rangle \end{array} \right\}$$

$$t = \langle B\sigma \vec{R} | H | A\sigma \vec{R} \rangle$$

3 fold rotation

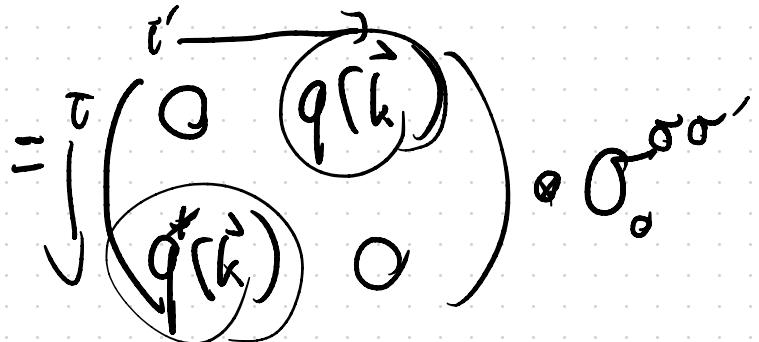
$$t = \langle B\sigma R - e_1 | H | A\sigma \vec{R} \rangle = \langle B\sigma \vec{R} - \vec{e}_1 | H | A\sigma \vec{R} \rangle$$

TRS: $t^* = t$

Inversion $t = \langle A\sigma \vec{R} | H | B\sigma \vec{R} \rangle = \langle A\sigma \vec{R} | H | B\sigma \vec{R} - \vec{e}_1 \rangle$
 $= \langle A\sigma \vec{R} | H | B\sigma \vec{R} - \vec{e}_1 \rangle$

Fourier transforming

$$h(\vec{k}) = \sum_{\vec{R}} e^{-i\vec{k} \cdot (\vec{R} + \vec{r}_\tau - \vec{r}_{\tau'})} S_{\sigma\sigma'} \langle \tau \sigma \vec{R} | H | \tau' \sigma' \vec{R} \rangle$$



$$q(\vec{k}) = t \left[e^{\frac{-2\pi i}{3}(k_1+k_2)} + e^{\frac{2\pi i}{3}(2k_1-k_2)} + e^{\frac{2\pi i}{3}(2k_2-k_1)} \right]$$

$$\text{Energies: } E_{\pm}(\vec{k}) = \pm |q(k)|$$

Three special values:

$$T: q(T) = 3t \quad h(T) = 3t \tau_x \sigma_0$$

$$E_{\pm}(T) = \pm 3t$$

$$K: k_1 = \frac{2}{3} \quad q(K) = t \left[e^{\frac{-2ij}{3}} + e^{\frac{2ij}{3}} + 1 \right] = 0$$

$$k_2 = \frac{1}{3}$$

$$E_{\pm}(K) = 0$$

$$M: k_1 = \frac{1}{2} \quad k_2 = 0 \quad q(M) = t \left[\frac{1}{2} - i\frac{\sqrt{3}}{2} \right]$$

$$h(M) = t \left(\frac{1}{2} T_x + \frac{\sqrt{3}}{2} T_y \right) \sigma_0$$

$$\epsilon_{\pm} = \pm t$$

