Assignment 12

Chiral vs Quantum Spin Hall insulators.

RISHI PARESH JOSHI

2111093

Problems from Topological Quantum Materials Concepts, Models, and Phenomena by Grigory Tkachov

Section 2.6

1) Given Hamiltonian for chern insulator:

$\hat{H}_{\vec{k}} = \vec{d}_{\vec{k}} \hat{I}_{2\times2} \cdot \vec{\hat{\sigma}}$ ①, where $I_{2\times2}$ is a 2×2 identity matrix & $\vec{\sigma}$ are the Pauli matrices.

$\vec{d}_{\vec{k}} = (\hbar v k_x, -\hbar v k_y, m)$ ②, where v is the fermi velocity & $k_{x/y}$ is the canonical momentum.

We need to show that,

(a) Edge modes are given by: $E(k) = -\,\mathrm{sgn}(m)\,\hbar v$ ③

(b) Berry connection components are:

$A^{(k)}_{\vec{k},s} = 0 \qquad A^{(\phi)}_{\vec{k},s} = -\left(\frac{1 - s\,u_z}{2k}\right)$ ④, where $u_z = \frac{\vec{d}_{\vec{k}}}{|\vec{d}_{\vec{k}}|}$

(c) Berry phase is :

$$\gamma_s = \oint \vec{A}_{k,s} \cdot d\vec{k} = -\pi(1 - s\,u_z) \quad (5)$$

(d) Berry curvature is:

$$\left(\vec{\nabla} \times \vec{A}_{\vec{k},s}\right)_z = \frac{s}{2k} \frac{\partial u_z}{\partial k} \quad (6)$$

(e) Relation to the Chern insulator hamiltonian with:

$$\vec{d}_{\vec{k}} = (\hbar v k_x, \hbar v k_y, m) - (7)$$

Solution:

Writing Hamiltonian in eqn 1 in polar coordinates:

$$k_x = k\cos\phi, \qquad k_y = k\sin\phi,$$

$$\vec{u}_{\vec{k}} = \frac{\vec{d}_{k}}{|d_{\vec{k}}|} = \frac{1}{\sqrt{(\hbar v k)^2 + m^2}}\left(\hbar v k\cos\phi, -\hbar v k\sin\phi, m\right) \quad (\text{From } 2)$$

Define:

$$u_z = \frac{m}{\sqrt{(\hbar v k)^2 + m^2}}, \quad u_{\parallel} = \sqrt{1 - u_z} = \frac{\hbar v k}{\sqrt{(\hbar v k)^2 + m^2}}$$

$$\vec{u}_{\vec{k}} = \left(u_{\parallel}\cos\phi, -u_{\parallel}\sin\phi, u_z\right).$$

This mean our Hamiltonian in eqn ① can be written as:

$$\hat{H}_{\vec{k}} = |\vec{d}_{\vec{k}}| \left(\vec{u}_{\vec{k}}\ \hat{I}_{2\times 2}\right) \cdot \vec{\hat{\sigma}}$$

$$\left(\vec{u}_{\vec{k}}\ \hat{I}_{2\times2} \cdot \vec{\hat{\sigma}}\right) = u_{\parallel} \cos\phi \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{\sigma_x} + (-u_{\parallel} \sin\phi) \underbrace{\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}}_{\sigma_y} + u_z \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}}_{\sigma_z}$$

$$\Rightarrow \left(\vec{u}_{\vec{k}}\ \hat{I}_{2\times2} \cdot \vec{\hat{\sigma}}\right) = \begin{bmatrix} u_z & u_{\parallel}\cos\phi + i\, u_{\parallel} \sin\phi \\ u_{\parallel}\cos\phi - i\, u_{\parallel}\sin\phi & -u_z \end{bmatrix} = \begin{bmatrix} u_z & u_{\parallel} e^{i\phi} \\ u_{\parallel} e^{-i\phi} & -u_z \end{bmatrix} \quad (8)$$

We now find the eigenvalues & hence the eigen vectors:

$$\Rightarrow (\lambda - u_z)(\lambda + u_z) - u_{\parallel}^2 = 0 \qquad \text{(From characteristic eqn)}$$

$$\Rightarrow \lambda^2 - (u_z^2 + u_{11}^2) = 0 \qquad \lambda = \pm\sqrt{u_z^2+u_{11}^2} = s\sqrt{u_z^2+u_{11}^2}$$

$$\Rightarrow E_{\vec{k},\text{bulk}} = |\vec{d}_{\vec{k}}|\lambda = s\sqrt{(\hbar v k)^2+m^2} \times \sqrt{\frac{m^2+(\hbar v k)^2}{m^2+(\hbar v k)^2}} = s\sqrt{(\hbar v k)^2+m^2}$$

(a) This is the bulk band structure. To find the edge modes, we write eqn (1) subs $k_x \to -i\partial_x$, $k_y \to -i\partial_y$:

$$E\psi(x,y) = \left[-i\hbar v\left(\hat{\sigma}_x\partial_y - \hat{\sigma}_y\partial_y\right) + m\hat{\sigma}_z\right]\psi(x,y)$$

Taking the ansatz: $\vec{\psi}(x,y) = \vec{\phi}(x,y)\, e^{ikx + y/\lambda}$, $\vec{\phi}$ is 2x2 with real entries.

$$E\,\vec{\phi}(x,y) = \hbar v k\,\hat{\sigma}_x\vec{\phi} + \left(\frac{i\hbar v}{\lambda}\hat{\sigma}_y + m\hat{\sigma}_z\right)\vec{\phi}$$

Separating the real & complex parts:

$$\Rightarrow E\vec{\Phi} = \hbar v k \hat{\sigma}_x \vec{\Phi} \qquad - \text{(I)} \quad \text{(Energy is real)}$$

$$\left(i\frac{\hbar v}{\lambda}\hat{\sigma}_y + m\hat{\sigma}_z\right)\vec{\Phi} = 0$$

Since $\sigma_z \cdot \sigma_x = i\sigma_y$,

$$\hat{\sigma}_z\left(\frac{\hbar v}{\lambda}\hat{\sigma}_x + m\right)\vec{\Phi} = 0$$

If $\vec{\Phi}$ is an eigenstate of σ_x,

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \rightarrow \underset{(S_x)}{\text{eigenvalues}} \in \{\pm 1\}, \text{ eigenvectors} \in \left\{\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \end{bmatrix}\right\}.$$

$$\hat{\sigma}_x\vec{\Phi} = S_x\vec{\Phi} \Rightarrow \left(\frac{\hbar v}{\lambda}S_x + m\right)\vec{\Phi} = 0 \Rightarrow S_x = -\frac{m\lambda}{\underbrace{\hbar v}_{+ve}}$$

Since $S_x = \pm 1$, $\lambda > 0$, $\quad S_x = -\operatorname{sgn}(m)$

$$\Rightarrow \; -\,\mathrm{sgn}(m) = -\frac{m\lambda}{\hbar v} \;\Rightarrow\; \lambda = \frac{\hbar v}{|m|} > 0.$$

This ensures as $y \to -\infty$, the wavefunction decays exponentially.

$$E\vec{\Phi} = \hbar v k \,\hat{\sigma}_x \vec{\Phi} = -\hbar v k \,\mathrm{sgn}(m)\,\vec{\Phi}$$

$$\Rightarrow \boxed{E_{k,\mathrm{edge}} = -\,\mathrm{sgn}(m)\,\hbar v k} \quad \text{matching Eq (3).}$$

(b) The eigenvectors of the hamiltonian (Eq (1)) & helicity operator (Eq (8)) are the same:

$$\begin{bmatrix} u_z & u_{\parallel} e^{i\phi} \\ u_{\parallel} e^{-i\phi} & -u_z \end{bmatrix} \to \underset{(s)}{\text{Eigenvalues}} \in \{\pm 1\}$$

$$\begin{bmatrix} u_z & u_{11}e^{i\phi} \\ u_{11}e^{-i\phi} & -u_z \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = s\begin{bmatrix} a \\ b \end{bmatrix}$$

$$\Rightarrow \quad u_z\, a + u_{11} e^{i\phi} b = sa$$

$$\Rightarrow \quad u_{11} e^{-i\phi} a - u_z b = sb$$

$$\Rightarrow \quad u_{11} e^{-i\phi} a = (s+u_z)\, b$$

$$\frac{a}{b} = \frac{(s+u_z)}{u_{11} e^{-i\phi}}$$

$$\Rightarrow \quad \vec{v} = \begin{pmatrix} s+u_z \\ u_{11} e^{-i\phi} \end{pmatrix}, \text{ where } \quad u_z = \frac{m}{\sqrt{(\hbar\omega k)^2 + m^2}}$$

On normalizing, $\quad c^2\left(u_{11}^2 + (s+u_z)^2\right) = 1$

$$c^2 = \frac{1}{u_{11}^2 + u_z^2 + 1 + 2su_z} = \frac{1}{2(1+su_z)}$$

$$c = \frac{1}{\sqrt{2(1+su_z)}}$$

$$\Rightarrow \psi_{k,s} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+su_z} \\ \frac{\sqrt{1-u_z^2}}{\sqrt{1+su_z}} e^{-i\phi} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+su_z} \\ \sqrt{\frac{(1-su_z)(1+su_z)}{(1+su_z)}}\, e^{-i\phi} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+su_z} \\ \sqrt{1-su_z}\, e^{-i\phi} \end{pmatrix}$$

$$\Rightarrow \vec{A}_{k,s} = -i \langle \psi_{k,s} | \vec{\nabla}_k | \psi_{k,s} \rangle$$

$$\Rightarrow A^{(k)}_{k,s} = -i \langle \psi_{k,s} | \partial_k | \psi_{k,s} \rangle , \qquad A^{(\phi)}_{k,s} = \frac{-i}{k} \langle \psi_{k,s} | \partial_\phi | \psi_{k,s} \rangle$$

$$\partial_\phi | \psi_{k,s} \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -i\sqrt{1-su_z}\, e^{-i\phi} \end{pmatrix}$$

$$\langle \psi_{k,s} | = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1+su_z} & , \sqrt{1-su_z}\, e^{i\phi} \end{pmatrix}$$

$$\boxed{\Rightarrow A^{(\phi)}_{k,s} = \frac{-i}{k} \langle \psi_{k,s} | \partial_\phi | \psi_{k,s} \rangle = -\frac{1}{2} \frac{(1-su_z)}{k}}$$

$$\partial_k \sqrt{1+s u_z} = \frac{1}{2} \frac{\partial_k u_z}{\sqrt{1+s u_z}} \quad , \quad \partial_k\left(\sqrt{1-s u_z}\right) = -\frac{1}{2} \frac{\partial_k u_z}{\sqrt{1-s u_z}}$$

$$\Rightarrow \quad \langle \psi_{k,s} | \partial_k | \psi_{k,s} \rangle = \frac{1}{2}\left[\sqrt{1+s u_z}\, \frac{\partial_k u_z}{\sqrt{1+s u_z}} + \sqrt{1-s u_z}\left(-\frac{\partial_k u_z}{\sqrt{1-s u_z}}\right)\right]$$

$$= 0$$

$$\Rightarrow \quad \boxed{A^{(k)}_{k,s} = 0 .}$$

(c) Berry phase:

$$\boxed{\gamma_s = \oint \vec{A}_{k,k} \cdot d\vec{k} = 2\pi k\, A^{(\phi)}_{k,s} = -\pi(1 - s u_z)}$$

(d) Berry curvature :

$$\left(\vec{\nabla}\times\vec{A}_{k,s}\right)_z = \frac{1}{k}\frac{\partial}{\partial k}\left(k A_{k,s}^{(\phi)}\right) = \frac{1}{k}\left(\frac{\partial}{\partial k}\left(-\frac{\cancel{k}}{2\cancel{k}}(1-s\,u_z)\right)\right)$$

$$\boxed{\left(\vec{\nabla}\times\vec{A}_{k,s}\right)_z = +\frac{s}{2k}\frac{\partial u_z}{\partial k}}$$

(e) The hamiltonian in Eq. 1 is the time reversed hamiltonian of the chern insulator hamiltonian (Eq. 7).

$$\vec{d}_{\vec{k}} = (\hbar v k_x, \hbar v k_y, m) \xrightarrow{TR} \vec{d}_{\vec{k}} = (\hbar v k_x, -\hbar v k_y, m)$$

TR $\rightarrow i\sigma_y K$ → Modern QM – Sakurai

K ← complex conjugation

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4) $$\hat{H}_{BHZ} = \begin{bmatrix} \hat{h}_k & 0 \\ 0 & \hat{h}^*_{-k} \end{bmatrix} \quad -(1)$$

BHZ → Bernevig, Hughes & Zhang Hamiltonian for HgTe/CdTe quantum wells

$$\hat{h}_k = A(\sigma_x k_x - \sigma_y k_y) + M_{\vec{k}}\sigma_z + D\vec{k}^2\sigma_0 \quad -(2)$$

& $$M_{\vec{k}} = M + B\vec{k}^2 \quad -(3)$$

where $\mathcal{A}$, $\mathcal{B}$, $\mathcal{D}$ and $\mathcal{M}$ are constants characterizing the band structure. Using the unitary transformation:

$$U = \begin{bmatrix} 0 & \sigma_z \\ -i\sigma_z & 0 \end{bmatrix} \quad \text{—(4)}$$

Obtain the Hamiltonian,

$$H'_{BHZ} = U\, H_{BHZ}\, U^{\dagger} \quad \text{—(5)}$$

and show that for

$$\mathcal{D} = \mathcal{B} = 0, \quad H'_{BHZ} = \begin{bmatrix} -i\hbar v(\sigma_x \partial_x + \sigma_y \partial_y) + \Delta\sigma_z & 0 \\ 0 & i\hbar v(\sigma_x \partial_x + \sigma_y \partial_y) - \Delta\sigma_z \end{bmatrix}$$

Eq. (6)

Solution:

Making $k \to -k$ and taking complex conjugate of Eq. (2),

$$\hat{h}^*_{-k} = \left[A\left(-\sigma_x k_x + \sigma_y k_y\right) + \left(M + B k^2\right)\sigma_z + D k^2 \sigma_0\right]^*$$

Since $\sigma_x^* = \sigma_x$, $\sigma_y^* = -\sigma_y$, $\sigma_z^* = \sigma_z$ & $\sigma_0^* = \sigma_0$,

$$\hat{h}^*_{-k} = \left[A^*\left(-\sigma_x k_x - \sigma_y k_y\right) + \left(M^* + B^* k^2\right)\sigma_z + D^* k^2 \sigma_0\right]$$

Thus, Eq. (1) is:

$$\hat{H}_{BHZ} = \begin{bmatrix} A(\sigma_x k_x - \sigma_y k_y) + (M^* + B^* k^2)\sigma_z + D^* k^2 \sigma_0 & 0 \\ 0 & A^*(-\sigma_x k_x - \sigma_y k_y) + (M^* + B^* k^2)\sigma_z + D^* k^2 \sigma_0 \end{bmatrix}$$

Now we define the unitary transformation :

$$\hat{U} = \begin{pmatrix} 0 & \sigma_z \\ -i\sigma_y & 0 \end{pmatrix} , \quad \hat{U}^+ = \begin{pmatrix} 0 & (-i\sigma_y)^+ \\ \sigma_z^{*+} & 0 \end{pmatrix} = \begin{pmatrix} 0 & i\sigma_y \\ \sigma_z & 0 \end{pmatrix}$$

$$\hat{U}^+ \hat{U} = \begin{pmatrix} \sigma_z^2 & 0 \\ 0 & (-i\sigma_y)^2 \end{pmatrix}$$

$$(-i\sigma_y)^2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

$$(\sigma_z)^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

$$\hat{U}^{+} U = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$$

Now we compute the transformed matrix:

$$H'_{BHZ} = \hat{U}\,\hat{H}_{BHZ}\,\hat{U}^{+} = \begin{pmatrix} 0 & U_{12} \\ U_{21} & 0 \end{pmatrix}\begin{pmatrix} \hat{h}_k & 0 \\ 0 & \hat{h}^*_{-k} \end{pmatrix}\begin{pmatrix} 0 & U^{+}_{12} \\ U^{+}_{21} & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & U_{12} \\ U_{21} & 0 \end{pmatrix} \begin{pmatrix} 0 & \hat{h}_k U_{12}^{+} \\ \hat{h}^*_{-k} U_{21}^{+} & 0 \end{pmatrix}$$

$$= \begin{pmatrix} U_{12} \hat{h}^*_{-k} U_{21}^{+} & 0 \\ 0 & U_{21} \hat{h}_k U_{12}^{+} \end{pmatrix}$$

$$U_{12} \hat{h}^*_{-k} U_{21}^{+} = \sigma_z \hat{h}^*_{-k} \sigma_z$$

$$= \sigma_z \left[A^* (-\sigma_x k_x - \sigma_y k_y) + (M^* + B^* k^2) \sigma_z + D^* k^2 \sigma_0 \right] \sigma_z$$

Using properties of σ matrices,

$$\sigma_x \sigma_z = -i \sigma_y \quad , \quad \sigma_y \sigma_z = i \sigma_x$$

$$\left(H'_{BHZ}\right)_{11} = \sigma_z\left[A^*\left(i\sigma_y k_x - i\sigma_x k_y\right) + \left(M^* + \beta^* k^2\right)\sigma_0 + D^* k^2 \sigma_z\right]$$

$$= A^*\left[\left(\sigma_x k_x\right) + \left(\sigma_y k_y\right)\right] + \left(M^* + \beta^* k^2\right)\sigma_z + D^* k^2 \sigma_0$$

$$\left(H'_{BHZ}\right)_{22} = U_{21}\, \hat{h}_k\, U_{12}^\dagger$$

$$= \left(-i\sigma_y\right)\left[A\left(\sigma_x k_x - \sigma_y k_y\right) + \left(M + \beta k^2\right)\sigma_z + D\vec{k}^2\sigma_0\right]\left(i\sigma_y\right)$$

$$= \left(-i\sigma_y\right)\left[A\left[\left(-\sigma_z\right)k_x - i k_y\right] + \left(M + \beta k^2\right)\sigma_x + D\vec{k}^2\left(i\sigma_y\right)\right]$$

$$= A\left[-\sigma_x k_x - \sigma_y k_y\right] - \left(M + \beta k^2\right)\sigma_z + D k^2 \sigma_0$$

$$\Rightarrow \boxed{H'_{BH2} = \begin{bmatrix} \mathcal{A}^*\left[(\sigma_x k_x)+(\sigma_y k_y)\right]+(\mathcal{M}+\beta^* k^2)\,\sigma_z+\mathcal{D}^* k^2 \sigma_0 & 0 \\ 0 & \mathcal{A}\left[(-\sigma_x k_x)-(\sigma_y k_y)\right]-(\mathcal{M}+\beta k^2)\,\sigma_z+\mathcal{D} k^2 \sigma_0 \end{bmatrix}}$$

Setting $\mathcal{A} = \hbar v$, $\beta = 0$, $\mathcal{D} = 0$, $k_x = -i\partial_x$ $k_y = -i\partial_y$:
$\mathcal{M} = \Delta$

$$\boxed{H'_{BH2} = \begin{bmatrix} -i\hbar v(\sigma_x \partial_x + \sigma_y \partial_y) + \Delta\,\sigma_z & 0 \\ 0 & i\hbar v(\sigma_x \partial_x + \sigma_y \partial_y) - \Delta\,\sigma_z \end{bmatrix}}$$

Thus, we get back Eq. 6.