Symmetry Protection of Edge States in a 2D Topological Insulator

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Abstract

Investigate how time-reversal symmetry protects the gapless edge states in a 2D Z_2 topological insulator (like the Bernevig-Hughes-Zhang (BHZ) model).

1 Mathematical Derivation

1. Start with the effective four-band BHZ model Hamiltonian in 2D:

$$H(\mathbf{k}) = \begin{pmatrix} m(\mathbf{k}) & Ak_x & 0 & -Ak_y \\ Ak_x & -m(\mathbf{k}) & -Ak_y & 0 \\ 0 & -Ak_y & -m(\mathbf{k}) & -Ak_x \\ -Ak_y & 0 & -Ak_x & m(\mathbf{k}) \end{pmatrix},$$

where $m(\mathbf{k}) = M - B(k_x^2 + k_y^2)$.
Answer: 4×4 Hamiltonian in momentum space $k_\pm = (k_x + k_y)$ is written in a block diagonal form

$$H(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h^*(\mathbf{k}) \end{pmatrix}$$

where $h(\mathbf{k})$ is spin up and $h^*(-\mathbf{k})$ is spin down related by time reversal symmetry.
The model is defined as $|E, \uparrow\rangle, |H, \uparrow\rangle, |E, \downarrow\rangle, |H, \downarrow\rangle$
For spin up block $h(\mathbf{k})$:
This block couple: $|E, \uparrow\rangle, |H, \uparrow\rangle$

$$h(\mathbf{k}) = \begin{pmatrix} m(\mathbf{k}) & Ak_- \\ Ak_+ & -m(\mathbf{k}) \end{pmatrix}$$

where: $k\pm = k_x \pm k_y$ then substitute this to k_- and k_+. We will get

$$h(\mathbf{k}) = \begin{pmatrix} m(\mathbf{k}) & A(k_x - k_y) \\ A(k_x + k_y) & -m(\mathbf{k}) \end{pmatrix}$$

For spin downt this block couple: $|E, \downarrow\rangle, |H, \downarrow\rangle$

$$h * (-\mathbf{k}) = \begin{pmatrix} -m(\mathbf{k}) & -Ak_+ \\ -Ak_- & m(\mathbf{k}) \end{pmatrix}$$

Substitute $k\pm = k_x \pm k_y$ to k_- and k_+. We will get

$$h(\mathbf{k}) = \begin{pmatrix} -m(\mathbf{k}) & -A(k_x - k_y) \\ -A(k_x + k_y) & m(\mathbf{k}) \end{pmatrix}$$

The given matrix for Hamiltonian is

$$H(\mathbf{k}) = \begin{pmatrix} m(\mathbf{k}) & Ak_x & 0 & -Ak_y \\ Ak_x & -m(\mathbf{k}) & -Ak_y & 0 \\ 0 & -Ak_y & -m(\mathbf{k}) & -Ak_x \\ -Ak_y & 0 & -Ak_x & m(\mathbf{k}) \end{pmatrix},$$

We can write this in spin system matrix

$$H(\mathbf{k}) = \begin{pmatrix} m(\mathbf{k}) & Ak_- & 0 & 0 \\ Ak_+ & -m(\mathbf{k}) & 0 & 0 \\ 0 & 0 & -m(\mathbf{k}) & -Ak_+ \\ 0 & 0 & -Ak_- & m(\mathbf{k}) \end{pmatrix},$$

Why is that the $-Ak_y$ in the diagonal becomes 0?
$*$ The $-Ak_y$ does not becomes zero. Since BHZ model does not include spin-flip terms. Primarily due to no coupling between spin-up and spin-down in the BHZ model.

2. Identify the time-reversal symmetry operator Θ for this system: $\Theta = \tau_0 \otimes i\sigma_y K$, where K is complex conjugation.
Answer: The time reversal operator

$$\Theta = \tau_0 \otimes (i\sigma_y)K$$

Where:
•τ_0 : 2×2 identity matrix in orbital space
•σ_y : acts in spin space
•K: Complex conjugation
The BHZ Hamiltonian uses the basis

$$|E, \uparrow\rangle, |H, \uparrow\rangle, |E, \downarrow\rangle, |H, \downarrow\rangle$$

Time Reversal Symmetry implies

$$\Theta H(k)\Theta^{-1} = H(-k)$$

We know that the 2×2 BHZ Hamiltonian diagonal block is

$$H(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h^*(\mathbf{k}) \end{pmatrix}$$

Where

$$h(\mathbf{k}) = \begin{pmatrix} m(\mathbf{k}) & Ak_- \\ Ak_+ & -m(\mathbf{k} \end{pmatrix}$$

For spin-up and $h^*(-k)$ is its time reversed counterpart Let's apply Θ and Θ^{-1} to H(k)

$$\begin{aligned} \Theta H(k)\Theta^{-1} &= (\tau_0 \otimes (i\sigma_y))K(H(k))K^{-1}(\tau_0 \otimes (-i\sigma_y)) \\ &= (\tau_0 \otimes (i\sigma_y))H^*(k)(\tau_0 \otimes (-i\sigma_y)) \end{aligned}$$

Take the complex conjugate

$$H^*(\mathbf{k}) = \begin{pmatrix} h^*(\mathbf{k}) & 0 \\ 0 & h(-\mathbf{k}) \end{pmatrix}$$

Then:

$$\Theta H^*(k)\Theta^{-1} = \begin{pmatrix} \sigma_y h^*(\mathbf{k})\sigma_y & 0 \\ 0 & \sigma_y h(-\mathbf{k})\sigma_y \end{pmatrix}$$

Using this identity

$$\sigma_y (d \cdot \sigma)^* \sigma_y = -d \cdot \sigma$$

Thefore

$$\sigma_y(h^*(k))\sigma_y = h(-k)$$
$$\sigma_y(h(-k))\sigma_y = h^*(-k)$$

So

$$\Theta H(k)\Theta^{-1} = \begin{pmatrix} h^*(\mathbf{k}) & 0 \\ 0 & h(-\mathbf{k}) \end{pmatrix}$$
$$\Theta H(k)\Theta^{-1} = H(-k)$$

Thus, the BHZ Hamiltonian is invariant under time reversal.

3. Analyze the bulk band structure and demonstrate the topological nature of the insulating phase by calculating the Z_2 topological invariant.
   Answer: The bulk Hamiltonian in the BHZ model(in momentume space) is:

$$H(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h^*(-\mathbf{k}) \end{pmatrix}$$

Each $h(k)$ is a 2×2:

$$h(k) = d(k) \cdot \sigma$$
$$h(k) = d_x(k) \cdot \sigma_x + d_y(k) \cdot \sigma_y + d_z(k) \cdot \sigma_z$$

Where:

$$d_x(k) = Asink_x$$
$$d_y(k) = Asink_y$$
$$d_x(k) = M - B(cosk_x + cosk_y)$$

•A: coupling parameter
•M: mass term
•B: band inversion control
Note: This model assumes a square lattice with lattice constant $a = 1$
For Bulk Band Structure
To find the energy bands diagonalize hk

$$E(k) = \pm|d(k)|$$
$$E(k) = \pm\sqrt{A^2(sin^2k_x + sin^2k_y) + [M - B(cosk_x + cosk_y)]}$$

This gives two bands per spin sector. The bandsare gapped as long as $E(k) \neq 0$ for all k in the brillouin zone

For the time reversal invariant systems in 2d. The Z_2 invariant can be computed from parity eigenvalues at the time reversal invariant momenta or TRIM
The TRIM points in 2D are:
$\Gamma = (0, 0)$
$X = (\pi, 0)$
$Y = (0, \pi)$
$M = (\pi, \pi)$

Fu and Kane's formula for inversion symmetry system is

$$(-1)^{\nu} = \prod_{i=1}^{4} \delta_i$$

Where:

$$\delta_1 = \prod_{n \in \text{occ}} \xi_{2n}(\Lambda_i)$$

Where $\xi_{2n}(\Lambda_i)$ is the parity eigenvalue of the $2n^{th}$ occupied Kramers pair at TRIM Λ_i
For BHZ model, These values depend on the sign of the mass term at each TRIM:

$$d_z(k) = M - B(cosk_x + cosk_y)$$

$\bullet at(0, 0) : d_z = M - 2B$
$\bullet at(\pi, 0), (0, \pi) : d_z = M$
$\bullet at(\pi, \pi) : d_z = M + 2B$
For Topological Phase Condition
$\bullet If M/B < 0$:Trivial Insulator
$\bullet If 0 < M/B < 2$: Non Trivial Topological Insulator
Therefore, when M/B in the range $0 < M/B < 2$, the Z_2 invariant is

$$\nu = 1$$

indicating a quantum spin Hall Insulator

4. Consider a finite-size strip geometry with open boundary conditions.
Answer: We now consider the BHZ model on a finite strip geometry

that is infinite in the x-direction and finite in the y-direction. This models a 2D topological insulator with physical edges at $y = 0$ and $y = L$, and imposes open boundary conditions in the y-direction:

$$\Psi(0) = \Psi(L) = 0.$$

The BHZ Hamiltonian in momentum space is given by:

$$H(\mathbf{k}) = \begin{pmatrix} m(\mathbf{k}) & Ak_x & 0 & -Ak_y \\ Ak_x & -m(\mathbf{k}) & -Ak_y & 0 \\ 0 & -Ak_y & -m(\mathbf{k}) & -Ak_x \\ -Ak_y & 0 & -Ak_x & m(\mathbf{k}) \end{pmatrix},$$

where the mass term is:

$$m(\mathbf{k}) = M - B(k_x^2 + k_y^2).$$

Due to spin conservation, the Hamiltonian is block diagonal and can be decomposed into two 2×2 blocks. Focusing on the spin-up block, we write the Hamiltonian in real space by replacing $k_y \to -i\partial_y$:

$$H_\uparrow(k_x, -i\partial_y) = \begin{pmatrix} M - B(k_x^2 - \partial_y^2) & A(k_x - i\partial_y) \\ A(k_x + i\partial_y) & -M + B(k_x^2 - \partial_y^2) \end{pmatrix}.$$

This results in a one-dimensional eigenvalue problem along the y-direction:

$$H_\uparrow(k_x, -i\partial_y)\Psi(y) = E\Psi(y),$$

where k_x acts as a good quantum number due to translational symmetry in the x-direction.

The goal is to find solutions $\Psi(y)$ that are localized near the boundaries and lie within the bulk energy gap. These are the topologically protected edge states.

5. Analytically derive the dispersion relation of the edge states that appear within the bulk band gap.
   Answer: We now derive the dispersion relation for the edge states that appear within the bulk energy gap of the BHZ model in a strip geometry. We focus on one spin block of the BHZ Hamiltonian, which in the continuum limit reads:

$$H(k_x, k_y) = A(k_x\sigma_x + k_y\sigma_y) + m(k)\sigma_z,$$

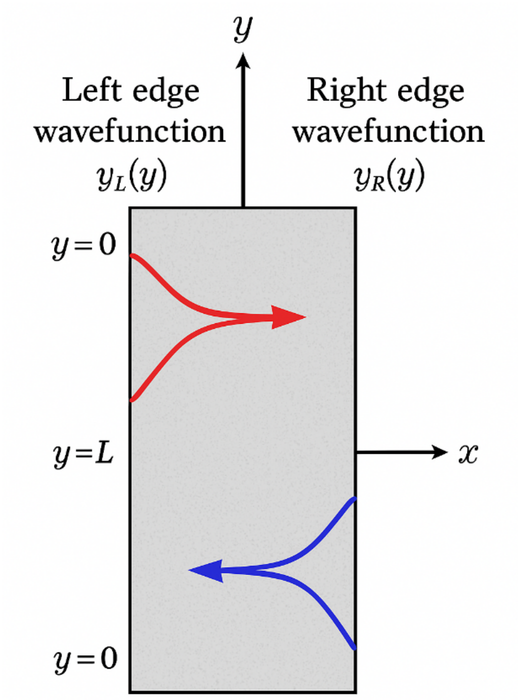

Figure 1: Strip Geometry

with mass term:

$$m(k) = M - B(k_x^2 + k_y^2).$$

In the strip geometry, x remains translationally invariant, while y is finite with open boundary conditions. We thus replace $k_y \to -i\partial_y$, leading to:

$$H(k_x, -i\partial_y) = A(k_x\sigma_x - i\partial_y\sigma_y) + [M - B(k_x^2 - \partial_y^2)]\sigma_z.$$

We seek edge-localized solutions using the ansatz:

$$\Psi(y) = e^{\lambda y}\chi, \quad \text{with } \operatorname{Re}(\lambda) < 0.$$

Applying the Hamiltonian to this wavefunction yields the eigenvalue equation:

$$\left[A(k_x\sigma_x - i\lambda\sigma_y) + (M - B(k_x^2 - \lambda^2))\sigma_z\right]\chi = E\chi.$$

This can be written explicitly as:

$$H_\lambda(k_x) = \begin{pmatrix} m_\lambda & A(k_x - \lambda) \\ A(k_x + \lambda) & -m_\lambda \end{pmatrix}, \quad \text{where } m_\lambda = M - B(k_x^2 - \lambda^2).$$

The eigenvalue equation leads to:

$$E^2 = A^2(k_x^2 - \lambda^2) + m_\lambda^2.$$

To obtain edge states, we consider a superposition of two exponentially decaying solutions:

$$\Psi(y) = c_1 e^{\lambda_1 y}\chi_1 + c_2 e^{\lambda_2 y}\chi_2,$$

with $\mathrm{Re}(\lambda_{1,2}) < 0$, and impose the boundary condition $\Psi(0) = 0$, which requires χ_1 and χ_2 to be linearly independent.

Edge states exist when E lies in the bulk band gap. For small k_x, this yields a linear dispersion:

$$E(k_x) = \pm A k_x.$$

This describes helical edge states that propagate in opposite directions for opposite spins. These modes are topologically protected and remain gapless as long as time-reversal symmetry is preserved.

6. Mathematically show how time-reversal symmetry enforces the Kramers degeneracy of the edge states at any momentum k and prevents backscattering between counter-propagating edge states with opposite spin, thus protecting their gaplessness.
Answer: We now derive the dispersion relation for the edge states that appear within the bulk energy gap of the BHZ model in a strip geometry. We focus on one spin block of the BHZ Hamiltonian, which in the continuum limit reads:

$$H(k_x, k_y) = A(k_x\sigma_x + k_y\sigma_y) + m(k)\sigma_z,$$

with mass term:

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This can be written explicitly as:

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The eigenvalue equation leads to:

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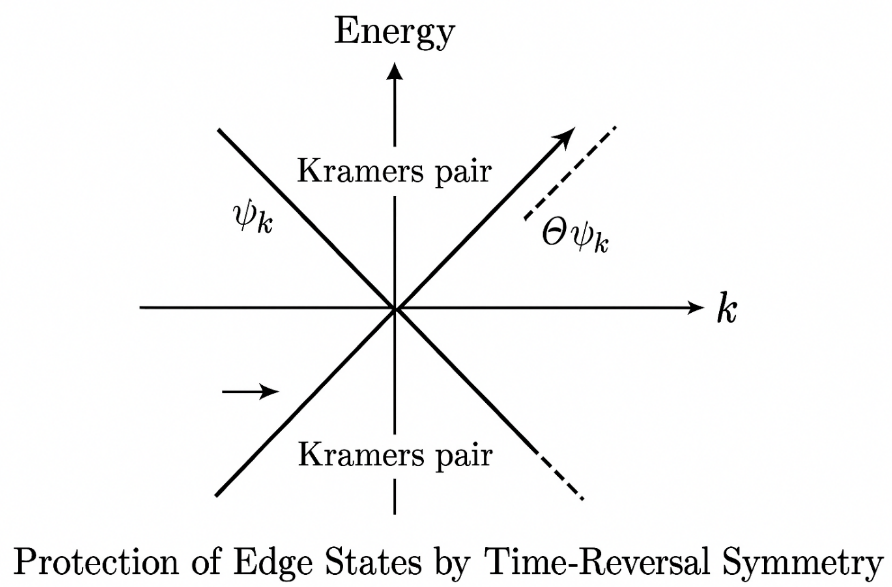

Figure 2: Protection of Edge State by Time Reversal Symmetry