Time-Reversal Symmetric Two-Dimensional Topological Insulators: The Bernevig-Hughes-Zhang Model

This notes are based on J.K. Asbóth, L. Oroszlány, A. Pályi. A Short Course on Topological Insulators ”http://arxiv.org/abs/1509.02295” (2015). and J.J. Sakurai. *Modern Quantum Mechanics*, (1994).

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Time Reversal Symmetry

We define a time reversal operator which acts as

$$|n\rangle \to \mathcal{T}|n\rangle$$

Where $\mathcal{T}|n\rangle$ is the time reversed state.
For example: if $|n\rangle = |\mathbf{k}\rangle$ we expect $\mathcal{T}|\mathbf{k}\rangle = |-\mathbf{k}\rangle$; if $|n\rangle = |\mathbf{x}\rangle$ we expect $\mathcal{T}|\mathbf{x}\rangle = |\mathbf{x}\rangle$.
We also say a Hamiltonian H has time reversal symmetry if $\mathcal{T}H\mathcal{T}^{-1} = H$.

How do we define this in a rigorous way?

Time Reversal Symmetry

The infinitesimal time evolution of a state $|n\rangle$ is generated by the Hamiltonian, and is given by

$$|n, t_0 = 0; t = \delta t\rangle = \left(1 - \frac{iH}{\hbar}\delta t\right)|n\rangle$$

If we consider applying the several operator at $t = 0$, then time evolving the state, then at $t = \delta t$ we have $\left(1 - \frac{iH}{\hbar}\delta t\right)\mathcal{T}|n\rangle$. Intuitively we expect that this should equal $\mathcal{T}|n, t_0 = 0; t = -\delta t\rangle$. Together this gives

$$\left(1 - \frac{iH}{\hbar}\delta t\right)\mathcal{T}|n\rangle = \mathcal{T}\left(1 - \frac{iH}{\hbar}(-\delta t)\right)|n\rangle$$

If this is to be true for any state $|n\rangle$ we find

$$-iH\mathcal{T}|n\rangle = \mathcal{T}iH|n\rangle$$

Time Reversal Symmetry

So we found:

$$-iH\mathcal{T}|n\rangle = \mathcal{T}iH|n\rangle$$

If $\mathcal{T}$ was a unitary operator then we may directly cancel the i's and find $-H\mathcal{T} = \mathcal{T}H$.
This does not work: as it implies

$$H\mathcal{T}|n\rangle = -\mathcal{T}H|n\rangle = -\epsilon_n\mathcal{T}|n\rangle$$

Therefore we find that the time reversal operator must be anti unitary ($\mathcal{T}c|n\rangle = c^*\mathcal{T}|n\rangle$, where $c \in \mathbb{C}$), this means

$$\mathcal{T}H = H\mathcal{T}$$

Time Reversal Symmetry

What is the effect of time reversal on the wave function?

$$\begin{aligned}\mathcal{T}|n\rangle &= \int d^3x' \mathcal{T}\big(|x'\rangle\langle x'|n\rangle\big) \\ &= \int d^3x' \mathcal{T}|x'\rangle\langle x'|n\rangle^* \\ &= \int d^3x' |x'\rangle\langle x'|n\rangle^*\end{aligned}$$

$$\begin{aligned}\mathcal{T}|n\rangle &= \int d^3k' \mathcal{T}\big(|k'\rangle\langle k'|n\rangle\big) \\ &= \int d^3k' \mathcal{T}|k'\rangle\langle k'|n\rangle^* \\ &= \int d^3k' |-k'\rangle\langle k'|n\rangle^* \\ &= \int d^3k' |k'\rangle\langle -k'|n\rangle^*\end{aligned}$$

So this shows that $\mathcal{T}\psi(x') \to \psi(x')^*$ and $\mathcal{T}\psi(p') \to \psi(-p')^*$.

The representation we choose crucially matters! We also see that two successive applications gives $\mathcal{T}^2 = 1$.
We will now show that this story differs for spinfull particles.

Time Reversal Symmetry

The spin eigenstates of a spin half particle can be written as $|\hat{\mathbf{n}},+\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y\beta/\hbar}|+\rangle$ and $|\hat{\mathbf{n}},-\rangle = e^{-iS_z\alpha/\hbar}e^{-iS_y(\pi+\beta)/\hbar}|-\rangle$. Now, noting that $\mathcal{T}|\hat{\mathbf{n}},+\rangle = |\hat{\mathbf{n}},-\rangle$ we deduce

$$\mathcal{T} = \eta e^{-i\pi J_y/\hbar}K$$

$$\begin{aligned}\mathcal{T}\big(\mathcal{T}\sum|j,m\rangle\langle j,m|n\rangle\big) &= \mathcal{T}\big(\eta\sum e^{-i\pi J_y/\hbar}|j,m\rangle\langle j,m|n\rangle^*\big)\\ &= |\eta|^2\sum e^{-2i\pi J_y/\hbar}|j,m\rangle\langle j,m|n\rangle\end{aligned}$$

Using the properties of the angular momentum eigenstates under rotation we note $e^{-2i\pi J_y/\hbar}|j,m\rangle = (-1)^{2j}|j,m\rangle$, therefore we find

$$\mathcal{T}^2|j\,\text{half-integer}\rangle = -\,|j\,\text{half-integer}\rangle$$
$$\mathcal{T}^2|j\,\text{integer} = +\,|j\,\text{integer}\rangle$$

Kramers Degeneracy

If we consider a system of charged particles in a static electric field, with $V(\mathbf{x}) = e\phi(\mathbf{x})$ then $[\mathcal{T}, H] = 0$ will still holds as the electrostatic potential is a real function of the time-reversal operator $\mathbf{x}$.
We consider a state $|n\rangle$ and its time reversed parter $\mathcal{T}|n\rangle$, these must have the same energy - following $H\mathcal{T}|n\rangle = \mathcal{T}H|n\rangle = \epsilon_n\mathcal{T}|n\rangle$.

So are these the same state or different states?

Kramers Degeneracy

The states $|n\rangle$ and $\mathcal{T}|n\rangle$ can only differ by a phase η with $\eta = e^{i\delta}$.

$$\mathcal{T}|n\rangle = e^{i\delta}|n\rangle$$

Now applying $\mathcal{T}$ once more

$$\mathcal{T}^2|n\rangle = \mathcal{T}e^{i\delta}|n\rangle = e^{-i\delta}\mathcal{T}|n\rangle = e^{-i\delta}e^{i\delta}|n\rangle = +|n\rangle$$

Which cannot hold for spin one-half particle. So we must conclude that these are different degenerate states.

This holds as long at the system obeys time-reversal symmetry!

Time Reversal Symmetry of Bulk Hamiltonian

Earlier we noted that $\mathcal{T}\psi(p') \to \psi(-p')^*$. It is also useful to realise we can split the time reversal operator into two parts $\mathcal{T} = \tau K$ where K is an operator which complex conjugates and τ is a unitary operator which acts on internal degrees of freedom.

$$\mathcal{T} H_{\text{Bulk}} \mathcal{T}^{-1} = \sum_{\mathbf{k}} |-\mathbf{k}\rangle\langle -\mathbf{k}| \otimes \mathcal{T} H(\mathbf{k}) \mathcal{T}^{-1} = \sum_{\mathbf{k}} |\mathbf{k}\rangle\langle \mathbf{k}| \otimes \tau H^*(-\mathbf{k}) \tau^{-1}$$

So $\tau H^*(-\mathbf{k})\tau^{-1} = H(\mathbf{k})$ in the TRS bulk, and therefore the Hamiltonian must be symmetric to inversion in the Brillouin zone.

The Bernevig-Hughes-Zhang model

How do we construct time reversal invariant Hamiltonians from a lattice model?
We take two copies of the system, where ones $H^* = KHK$ and couple in the same manner as we did with the Chern insulators.

$$H_{\text{TRI}} = \begin{pmatrix} H & C \\ C^\dagger & H^* \end{pmatrix}$$

The Bernevig-Hughes-Zhang model

We look for a coupling with $\mathcal{T}^2 = 1$. We have two options: we choose $\mathcal{T} = s_x K$.
This gives

$$s_x K H_{\text{TRI}} (s_x K)^{-1} = H_{\text{TRI}}$$

If we chose the coupling such that $C = C^T$.
Additionally we may choose an even simpler solution with $\mathcal{T} = K$ and not even double the Hilbert space

$$H_{\text{TRI}} = \frac{H + H^*}{2} = K H_{\text{TRI}} K$$

The Bernevig-Hughes-Zhang model

We look for a coupling with $\mathcal{T}^2 = -1$, therefore we choose $\mathcal{T} = is_y K$. This gives

$$is_y K H_{\text{TRI}} (is_y K)^{-1} = H_{\text{TRI}}$$

If we chose the coupling such that $C = -C^T$.

So we see different types of TRS must be satisfied by different couplings.

The Bernevig-Hughes-Zhang model

We now introduce a toy model for a time-reversal invariant topological insulator.

$$H_{\mathrm{BHZ}}(\mathbf{k}) = s_0 \otimes \left[(u + \cos k_x + \cos k_y)\sigma_z + \sin k_y \sigma_y\right] + s_z \otimes \sin k_x \sigma_x + s_x \otimes \hat{C}$$

For $C = 0$ this reduces to a 4 band model of HgTe.

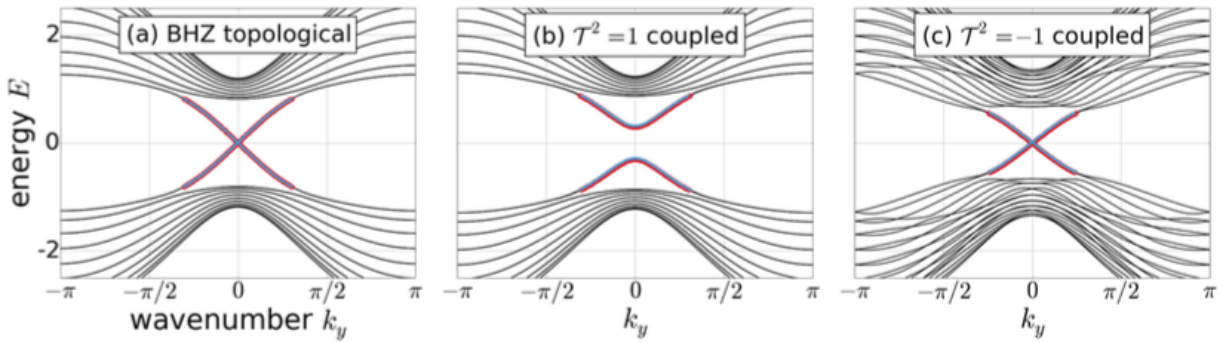
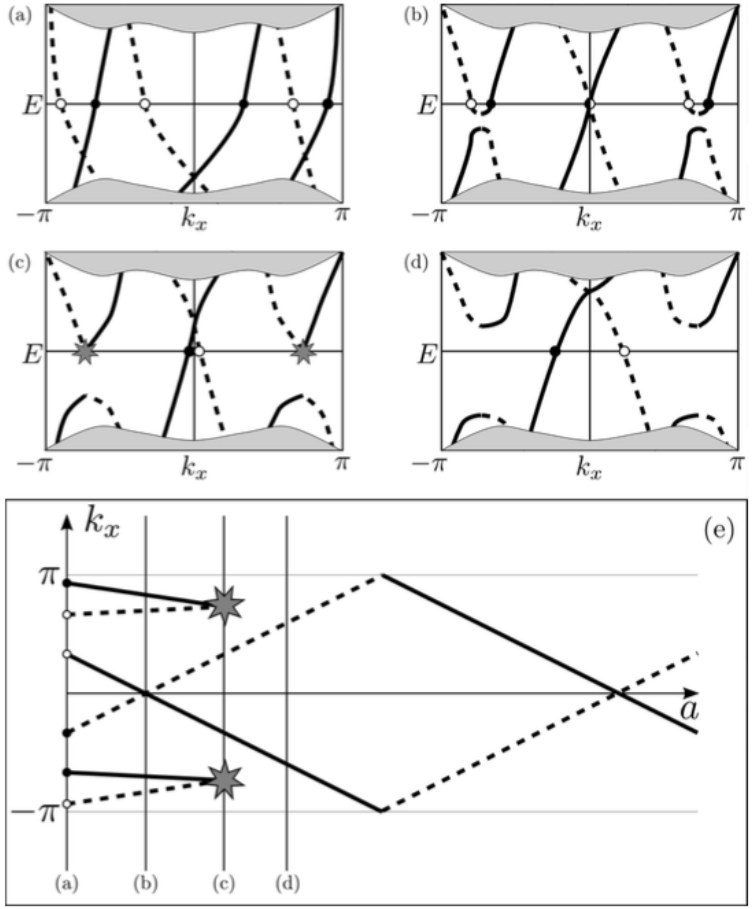


Fig. 8.1 Stripe dispersion relations of the BHZ model, with sublattice potential parameter $u = -1.2$. Right/left edge states (more than 60% weight on the last/first two columns of unit cells) marked in dark red/light blue. (a): uncoupled layers, $\hat{C} = 0$. (b): Symmetric coupling $\hat{C} = 0.3\sigma_x$ gaps the edge states out. (c): Antisymmetric coupling $\hat{C} = 0.3\sigma_y$ cannot open a gap in the edge spetrum.

Edge States



The $\mathbb{Z}_2$ invariant

$\mathcal{T}^2 = -1$ demands that we have and equal number of left movers and right moves at any given energy in the bulk gap.

$$N_+(E) = N_-(E)$$

Due to Kramers degeneracy adiabatic deformations of the edge states can only change the number of edge states by 4, a pair of kramers pairs.
Therefore we define the $\mathbb{Z}_2$ as the party of the number of Kramers pairs, this is a topological invariant.

$\mathbb{Z}_2$ = 0(1) for even(odd) number of Kramers pairs.

Absence of Back Scattering

How does edge state transport behave under the influence of local disorder?

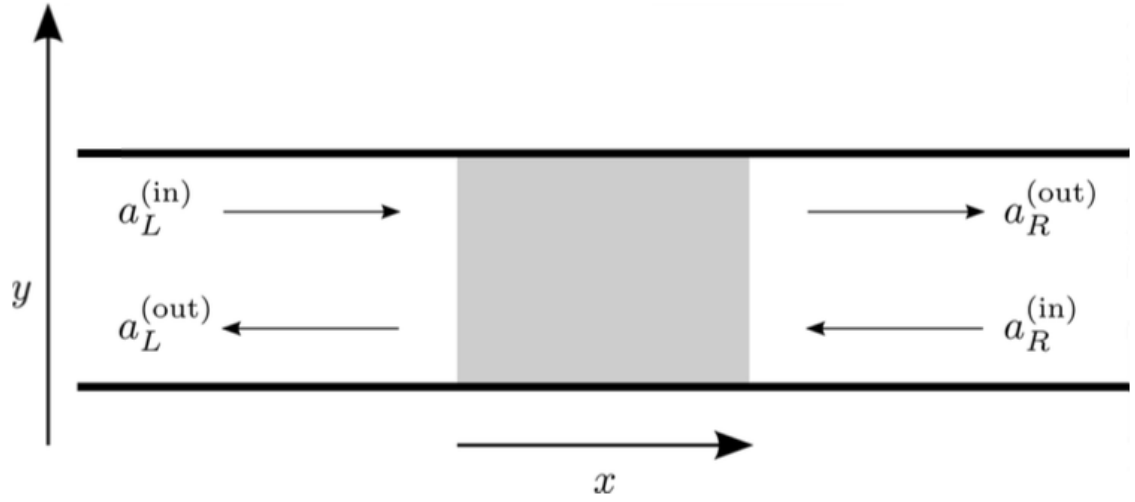


Fig. 8.3 Disordered region (gray) obstructing electrons in a two-dimensional phase-coherent conductor. The scattering matrix S relates the amplitudes $a_L^{(\mathrm{in})}$ and $a_R^{(\mathrm{in})}$ of incoming waves to the amplitudes $a_L^{(\mathrm{out})}$ and $a_R^{(\mathrm{out})}$ of outgoing waves.

Absence of Back Scattering

Consider a lattice model where the unit cells form a square lattice of size $N_x \times N_y$. If the system is translational invariant in the x-direction we may write the Bloch states as

$$|l\pm\rangle = |k_{l,\pm}\rangle \otimes |\Phi_{l,\pm}\rangle$$

where the momentum eigenstates are given by

$|k\rangle = \frac{1}{N_x}\sum_{m_x=1}^{N_x} e^{ikm_x}|m_x\rangle$ and $|\Phi_{l,\pm}\rangle$ incorporates the transverse modes and the sublattice degree of freedom.

We will use these current-normalised states defining

$|l\pm\rangle_c = \frac{1}{\sqrt{|v_{l,\pm}|}}|l\pm\rangle$ with $v_{l,\pm}$ being the group velocity.

Absence of Back Scattering

A wave incident on the scattering region is characterized by a vectors of coefficients, in the lead index L, R

$$a^{(\text{in})} = \left(a^{(\text{in})}_{L,1}, a^{(\text{in})}_{L,2}, ..., a^{(\text{in})}_{L,N}, a^{(\text{in})}_{R,1}, a^{(\text{in})}_{R,2}, ..., a^{(\text{in})}_{R,N}\right)$$

$$a^{(\text{out})} = \left(a^{(\text{out})}_{L,1}, a^{(\text{out})}_{L,2}, ..., a^{(\text{out})}_{L,N}, a^{(\text{out})}_{R,1}, a^{(\text{out})}_{R,2}, ..., a^{(\text{out})}_{R,N}\right)$$

The corresponding energy eigenstate reads

$$|\psi\rangle = \sum_{l=1}^{N} a^{(\text{in})}_{L,l}|l,+,L\rangle_c + a^{(\text{out})}_{L,l}|l,-,L\rangle_c + a^{(\text{in})}_{R,l}|l,-,R\rangle_c + a^{(\text{out})}_{L,l}|l,+,R\rangle_c$$

The scattering matrix S relates the two vectors

$$a^{(\text{out})} = Sa^{(\text{in})} \qquad S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

Absence of Back Scattering

Kramers degeneracy gives the connection between states.

$$|l,-,L\rangle_c = \mathcal{T}|l,+,L\rangle_c$$
$$|l,+,R\rangle_c = \mathcal{T}|l,-,R\rangle_c$$

We may write the eigenstates outside the scattering region as

$$|\psi\rangle = \sum_{l=1}^{N} a_{L,l}^{(\text{in})}|l,+,L\rangle_c + (Sa^{(\text{in})})_{L,l}|l,-,L\rangle_c$$
$$+ a_{R,l}^{(\text{in})}|l,-,R\rangle_c + (Sa^{(\text{in})})_{L,l}|l,+,R\rangle_c$$

Absence of Back Scattering

We now look for the time reversed state

$$-\mathcal{T}|\psi\rangle = \sum_{l=1}^{N} -a_{L,l}^{(\text{in})*}|l,-,L\rangle_c + (S^* a^{(\text{in})*})_{L,l}|l,+,L\rangle_c$$
$$- a_{R,l}^{(\text{in})*}|l,+,R\rangle_c + (S^* a^{(\text{in})*})_{L,l}|l,-,R\rangle_c$$

Comparing $|\psi\rangle$ and $-\mathcal{T}|\psi\rangle$ we must conclude

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} = -S^T = \begin{pmatrix} -r & -t \\ -t' & -r' \end{pmatrix}$$

We gives $r = -r$ therefore $r = 0$.