Symmetry Classifications of Topological Systems

This notes are based on a combination of J.K. Asbóth, L. Oroszlány, A. Pályi. A Short Course on Topological Insulators "http://arxiv.org/abs/1509.02295" (2015), J.J. Sakurai. *Modern Quantum Mechanics*, (1994), B.A. Bernevig, Topological Insulators and Topological Superconductors, Princeton University Press, (2013) and C-K. Chiu, J.C.Y. Teo, A.P. Schnyder and S. Ryu, Rev. Mod. Phys, 88, (2016).

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We define a time reversal operator which acts as

$$|n
angle o \mathcal{T}|n
angle$$

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?

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

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

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So we found:

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

If T was a unitary operator then we may directly cancel the *i*'s and find -HT = TH. 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

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

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

$$\mathcal{T}|n\rangle = \int d^{3}x' \mathcal{T}(|x'\rangle\langle x'|n\rangle) \qquad \mathcal{T}|n\rangle = \int d^{3}k' \mathcal{T}(|k'\rangle\langle k'|n\rangle)$$

$$= \int d^{3}x' \mathcal{T}|x'\rangle\langle x'|n\rangle^{*} \qquad = \int d^{3}k' \mathcal{T}|k'\rangle\langle k'|n\rangle^{*}$$

$$= \int d^{3}x'|x'\rangle\langle x'|n\rangle^{*} \qquad = \int d^{3}k'|-k'\rangle\langle k'|n\rangle^{*}$$

$$= \int d^{3}k'|k'\rangle\langle -k'|n\rangle^{*}$$

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 $T^2 = 1$.

We will now show that this story differs for spin-full particles.

If time reversal gives $TST^{-1} = -S$, then TRS rotates the spin by π . Choosing the axis of rotation to be about the y-axis we find

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

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

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

$$\mathcal{T}^2 | j \text{ half-integer}
angle = - | j \text{ half-integer}
angle$$

 $\mathcal{T}^2 | j \text{ integer}
angle = + | j \text{ integer}
angle$

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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?

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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!

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Time Reversal Symmetry of Bulk Hamiltonian

What happens to systems which in addition to TRS there exists also a translational symmetry?

Earlier we noted that $\mathcal{T}\psi(p') \rightarrow \psi(-p')^*$. It is also useful to realise we can split the time reversal operator into two parts $\mathcal{T} = \tau \mathcal{K}$ where \mathcal{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 (i.e. $\mathbf{k} \to -\mathbf{k}$).

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Time Reversal Symmetry of Bulk Hamiltonian

We can take an eigenstate of $H(\mathbf{k})$ as

$$H(\mathbf{k})|u(\mathbf{k})\rangle = E(\mathbf{k})|u(\mathbf{k})\rangle$$
 .

Using time reversal symmetry we obtain,

$$\tau H^*(-\mathbf{k})\tau^{-1}|u(\mathbf{k})\rangle = E(\mathbf{k})|u(\mathbf{k})\rangle$$

then, multiplying from left by τ^{-1} and taking the complex conjugate we find

$$H(-\mathbf{k})\tau^{T}|u(\mathbf{k})\rangle^{*} = E(\mathbf{k})\tau^{T}|u(\mathbf{k})\rangle^{*}$$

So for every eigenstate $|u(\mathbf{k})\rangle$ of $H(\mathbf{k})$ there is a time-reversed partner eigenstate of $H(-\mathbf{k})$ at the same energy at $\tau^T |u(\mathbf{k})\rangle^*$. This implies inversion symmetry of the energies, $E(\mathbf{k}) = E(-\mathbf{k})$. Note, however, that $E(\mathbf{k}) = E(-\mathbf{k})$ is not enough to guarantee time-reversal symmetry.

Vanishing of Hall Conductance for T Invariant Half-Integer Spin Systems

As we have noted in previous lectures, $\sigma_{xy} = \sigma_{yx} = 0$ for all systems with time reversal symmetry. Taking a rather brute force approach we consider the Berry Curvature $F(k_x, k_y)$ of a two occupied Bloch bands $|u_n(\mathbf{k})\rangle$ with n = I, II, we find

$$F(k_x, k_y) = (-i\langle \partial_{k_x} u_I(\mathbf{k}) | \partial_{k_y} u_I(\mathbf{k}) \rangle - x \leftrightarrow y) + I \leftrightarrow II \ .$$

After algebra we find

$$\begin{split} &\langle \partial_{-k_x} u_I(-\mathbf{k}) | \partial_{-k_y} u_I(-\mathbf{k}) \rangle - x \leftrightarrow y = - \langle \partial_{k_x} u_{II}(\mathbf{k}) | \partial_{k_y} u_{II}(\mathbf{k}) \rangle - x \leftrightarrow y \; . \\ &\langle \partial_{-k_x} u_{II}(-\mathbf{k}) | \partial_{-k_y} u_{II}(-\mathbf{k}) \rangle - x \leftrightarrow y = - \langle \partial_{k_x} u_I(\mathbf{k}) | \partial_{k_y} u_I(\mathbf{k}) \rangle - x \leftrightarrow y \; . \end{split}$$

Which implies $F(k_x, k_y) = -F(-k_x, -k_y)$, therefore this will always vanish upon integration over the whole Brillouin zone.

Charge Conjugation Symmetry

Charge conjugation or particle-hole symmetry is a unitary transformation that mixes electrons and holes. Indeed, in particle number conserving systems is acts to flip to sign of charge carriers.

We can demand the anticomutation relation $\{c_{i,\sigma}, c_{i,\sigma}^{\dagger}\} = \delta_{ij}$ is invariant. Here we see the particle-hole symmetry explicitly with $Cc_{i,\sigma}C^{-1} = c_{i,\sigma}^{\dagger}$ and $Cc_{i,\sigma}^{\dagger}C^{-1} = c_{i,\sigma}$.

Considering its action on a single-particle Hamiltonian we find

$$\mathcal{C}^{-1}H\mathcal{C} = -H$$

and therefore is not a unitary symmetry. In a similar way to TRS we can find $C^2 = \pm 1$ with -1 solution for half-integer states and +1 for integer states.

Charge Conjugation Symmetry

We can take an eigenstate of the single particle bulk Hamiltonian $H(\mathbf{k})$ as

$$H(\mathbf{k})|u(\mathbf{k})\rangle = E(\mathbf{k})|u(\mathbf{k})\rangle$$
.

Using charge conjugation symmetry $C = \mu \mathcal{K}$ we obtain,

$$-\mu H^*(-\mathbf{k})\mu^{-1}|u(\mathbf{k})\rangle = E(\mathbf{k})|u(\mathbf{k})\rangle$$

then, multiplying from left by μ^{-1} and taking the complex conjugate we find

$$H(-\mathbf{k})\mu^T |u(\mathbf{k})\rangle^* = -E(\mathbf{k})\mu^T |u(\mathbf{k})\rangle^*$$
.

So for every eigenstate $|u(\mathbf{k})\rangle$ of $H(\mathbf{k})$ there is a charge-conjugated partner eigenstate of $H(\mathbf{k})$ at the opposite energy $-E(\mathbf{k})$ at $\mu^{T}|u(\mathbf{k})\rangle^{*}$.

The combination of \mathcal{T} and \mathcal{C} gives rise to a third symmetry, chiral symmetry. Indeed, we can imagine a situation in which both \mathcal{T} and \mathcal{C} are absent but their combination is satisfied. So Chiral symmetry is given by

$$S = T \cdot C$$

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And for single particle Hamiltonians satisfies

$$\mathcal{S}^{-1}H\mathcal{S} = -H$$

As this is constructed of two anti unitary operators we find $\nu\nu^{-1} = 1$, i.e. only one solution.

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We now want a general classification of single particle Hamiltonians in terms of these symmetries.

$\mathcal{T}^{-1}H\mathcal{T}=H$	$\mathcal{T}= au\mathcal{K}$	$\tau\tau^*=\pm\mathbb{1}$
$\mathcal{C}^{-1}H\mathcal{C}=-H$	$\mathcal{C} = \mu \mathcal{K}$	$\mu\mu^* = \pm \mathbb{1}$
$\mathcal{S}^{-1}H\mathcal{S} = -H$	$\mathcal{S} = \nu$	$\nu^2 = \mathbb{1}$

Note that unitary symmetries, which commute with the Hamiltonian, allow us to bring the Hamiltonian into a block diagonal form. Here our aim is to classify the symmetry properties of these irreducible blocks, which do not exhibit any unitary symmetries.

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Class	Т	С	S	0	1	2	3	4	5	6	7
A	0	0	0	Z	0	Z	0	\mathbb{Z}	0	Z	0
AIII	0	0	1	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}	0	\mathbb{Z}
AI	+	0	0	\mathbb{Z}	0	0	0	2ℤ	0	\mathbb{Z}_2	\mathbb{Z}_2
BDI	+	+	1	\mathbb{Z}_2	\mathbb{Z}	0	0	0	$2\mathbb{Z}$	0	\mathbb{Z}_2^-
D	0	+	0	\mathbb{Z}_2^-	\mathbb{Z}_2	\mathbb{Z}	0	0	0	$2\mathbb{Z}$	0
DIII	_	+	1	0	$\mathbb{Z}_2^{}$	\mathbb{Z}_2	\mathbb{Z}	0	0	0	2ℤ
AII	_	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2^{\tilde{2}}$	\mathbb{Z}_2	\mathbb{Z}	0	0	0
CII	_	_	1	0	$2\mathbb{Z}$	0	\mathbb{Z}_2^-	\mathbb{Z}_2	\mathbb{Z}	0	0
С	0	_	0	0	0	2ℤ	Õ	$\mathbb{Z}_2^{}$	\mathbb{Z}_2	\mathbb{Z}	0
CI	+	-	1	0	0	0	2ℤ	0	$\mathbb{Z}_2^{}$	\mathbb{Z}_2	\mathbb{Z}

Alexander Pearce

Intro to Topological Insulators: Week 5

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An Example 1: The SSH model from lecture 1

$$H(k) = \mathbf{R}(k) \cdot \boldsymbol{\sigma} \quad ; \quad \mathbf{R}(k) = \begin{pmatrix} t - t' \cos k \\ -t' \sin k \\ 0 \end{pmatrix}$$

We find Hamiltonian has only chiral symmetry given by $\sigma_z H(k)\sigma_z = -H(k)$, and therefore is belongs to class AIII. Indeed, as we already knew, in one dimension it's topological phases are governed by a winding number \mathbb{Z} .

An Example 2: The QWZ model on a square lattice from lecture 4

$$H(k) = \mathbf{R}(k) \cdot \boldsymbol{\sigma} \; ; \; \mathbf{R}(k) = \left(\begin{array}{c} \sin k_x \\ \sin k_y \\ u + \cos k_x + \cos k_y \end{array} \right)$$

If σ refers to real spin then $R(-\mathbf{k}) = -R(\mathbf{k})$ for TRS to hold, therefore $R_z(\mathbf{k})$ being even breaks TRS. Now for σ being some isospin, $R_x(\mathbf{k})$ and $R_z(\mathbf{k})$ must be even in k and $R_y(\mathbf{k})$ odd in k. Therefore this is Class A, and as we already knew, in two dimension

it's topological phases are governed by a winding number \mathbb{Z} .

An Example 3: The B phase of superfluid ³He

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{k}} \Psi^{\dagger}(\mathbf{k}) H(\mathbf{k}) \Psi(\mathbf{k})$$

where

$$H(k) = \left(\begin{array}{cc} \xi({\bf k}) & \Delta({\bf k}) \\ \Delta^{\dagger}({\bf k}) & -\xi({\bf k}) \end{array} \right)$$

 $\Psi^{\dagger}(\mathbf{k}) = (\psi^{\dagger}_{\uparrow}, \psi^{\dagger}_{\downarrow}, \psi_{\uparrow}, \psi_{\downarrow}) \quad \xi(\mathbf{k}) = \mathbf{k}^2/2m - \mu \quad \Delta(\mathbf{k}) = \Delta_0 i \sigma_2 \mathbf{k} \cdot \boldsymbol{\sigma}$

This BdG Hamiltonian satisfies $\tau_1 H^T(\mathbf{k})\tau_1 = -H(\mathbf{k})$ and $\sigma_2 H^*(-\mathbf{k})\sigma_2$. (note all BdG Hamiltonian have particle-hole symmetry by construction)

Therefore this is Class DIII, and as we already knew, in three dimension its has topological nontrivial phases and is governed by a winding number \mathbb{Z} . ($\nu_3 = (1/2)(\text{sgn}[\mu] + 1)$)

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