

Experimental signature:

- IQHE: Quantized Hall conductivity (perfect quantization, error bar $1/10^9$).
- QSHE: Conductivity $= 2e^2/h$ (2 comes from the fact that we have two edge states). Notice that
 - 1. this is conductivity NOT Hall conductivity.
 - 2. this quantization is much less accurate (1% error bar for clear samples with very small size, very large deviation for larger samples or dirty samples). This is because the impurity scattering here is non-zero.

Interactions?

If we ignore the interactions and consider free fermions, IQHE and QSHE has little difference (the latter is just two copies of the former). However, if we consider interacting fermions:

- IQHE: We know that all the effect remain the same in the presence of strong interactions (in addition to the free fermion band structure theory, we also have the gauge theory, Green's function theory, and flux insertion techniques, which tell us that the Hall conductivity will remain integer-valued, even if we have very strong interactions in our system).
- QSHE: We don't have full understanding about interactions: What is the gauge theory describe (maybe BF theory)? Whether the conductivity is still $2e^2/h$ in the presence of strong interactions?.

3D

- IQHE: Can only happen in even dimensions 2, 4, 6 ... There is no IQHE in 3D.
- QSHE: Can be generalized to 3D

5.7. time-reversal symmetry for spin-1/2 and Kramers doublet

Q: How to write down the time-reversal operator for a spin-1/2 particle?

Basic knowledge:

- Spin 1/2: described by the Pauli matrices
- Time-reversal transformation is anti-unitary
- Time-reversal transformation change the sign of spin.

Define time-reversal operator

$$\mathcal{T} = U_T \theta \quad (5.27)$$

where U_T is an unitary matrix and θ is the operator for complex conjugate. ($\theta^{-1} = \theta$)

Because the time-reversal operator flips the sign of a spin, we have

$$\mathcal{T} \sigma_x \mathcal{T}^{-1} = -\sigma_x \quad \text{and} \quad \mathcal{T} \sigma_y \mathcal{T}^{-1} = -\sigma_y \quad \text{and} \quad \mathcal{T} \sigma_z \mathcal{T}^{-1} = -\sigma_z \quad (5.28)$$

$$U_T \theta \sigma_x \theta U_T^{-1} = -\sigma_x \quad \text{and} \quad U_T \theta \sigma_y \theta U_T^{-1} = -\sigma_y \quad \text{and} \quad U_T \theta \sigma_z \theta U_T^{-1} = -\sigma_z \quad (5.29)$$

$$\theta \sigma_x \theta = \theta \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \theta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \theta^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x \quad (5.30)$$

$$\theta \sigma_z \theta = \theta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \theta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \theta^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z \quad (5.31)$$

$$\theta \sigma_y \theta = \theta \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \theta = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \theta^2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} = -\sigma_y \quad (5.32)$$

$$U_T \sigma_x U_T^{-1} = -\sigma_x \quad \text{and} \quad U_T \sigma_y U_T^{-1} = \sigma_y \quad \text{and} \quad U_T \sigma_z U_T^{-1} = -\sigma_z \quad (5.33)$$

To satisfies these three relations, the only unitary matrix one can write down is

$$U_T = e^{i\phi} \sigma_y \quad (5.34)$$

where ϕ is an arbitrary phase, which depends on the choice of basis. The choice of ϕ has no physical consequence and doesn't change the value of any physical observables. Typically, people fix the value of ϕ by requiring U_T to be a real matrix ($\phi=\pi/2$ or $\phi=3\pi/2$). If we choose $\phi=\pi/2$

$$U_T = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (5.35)$$

$\mathcal{T}^2 = ?$

Q: In classical mechanics, if we flip the arrow of time twice, everything should go back to itself ($\mathcal{T}^2 = 1$). Is this also true for a quantum system?

A: For integer spins, $\mathcal{T}^2 = 1$, but for half-integer spins $\mathcal{T}^2 = -1$

Example: spin-1/2

$$U_T = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad (5.36)$$

$$\mathcal{T} = U_T \theta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \theta \quad (5.37)$$

$$\mathcal{T}^2 = U_T \theta U_T \theta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \theta \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \theta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \theta^2 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} = -I \quad (5.38)$$

$$\mathcal{T} |\psi\rangle = |\psi^*\rangle \quad (5.39)$$

$$\mathcal{T}^2 |\psi\rangle = \mathcal{T} |\psi^*\rangle = -|\psi\rangle \quad (5.40)$$

Flip the arrow of time twice, the wavefunction for a spin-1/2 particle changes sign.

We know that there is an arbitrary phase in $U_T = e^{i\phi} \sigma_y$. Let's now verify that the conclusion $\mathcal{T}^2 = -1$ is independent of the choice of ϕ

$$\mathcal{T}^2 = U_T \theta U_T \theta = e^{i\phi} \sigma_y \theta e^{i\phi} \sigma_y \theta = e^{i\phi} \sigma_y e^{-i\phi} (-\sigma_y) \theta^2 = -\sigma_y \sigma_y = -I \quad (5.41)$$

Still $\mathcal{T}^2 = -1$.

Q: What will happen if \mathcal{T} is an unitary transformation?

A: for unitary transformations, $O^2 = e^{2i\phi}$, which could take any value (depending on the choice of ϕ), so it makes no sense to consider the sign of

Let's drop the anti-unitary part θ , and consider the unitary operator:

$$O = U_T = e^{i\phi} \sigma_y \quad (5.42)$$

$$O^2 = e^{i\phi} \sigma_y e^{i\phi} \sigma_y = e^{2i\phi} \quad (5.43)$$

For unitary operators, the phase of O^2 is not well defined (depending on the choice of gauge), so we cannot talk about the sign of O^2 .

Bottom line: the sign of O^2 can only be defined for anti-unitary operators (like \mathcal{T} or the particle-hole transformation C)

Why $\mathcal{T}^2 = -1$ for spin 1/2?

This is not an rigorous proof. But what I am going to present to you shows that spin-1/2 is special and -1 is nature for particles with spin-1/2.

Q: What will happen if we rotate the spin of a spin-1/2 particle by 2π ?

Classical mechanics tells us that 2π rotation is like doing nothing. But this is NOT true for quantum mechanics.

A: For spin-1/2 particles, a 2π rotation is -1.

Define the rotation operator:

$$R_z(\theta) = \exp(-i S_z \theta / \hbar) = \exp(-i \sigma_z \theta / 2) = \cos \frac{\theta}{2} - i \sigma_z \sin \frac{\theta}{2} \quad (5.44)$$

For $\theta=2\pi$

$$R_z(2\pi) = \cos \frac{2\pi}{2} - i \sigma_z \sin \frac{2\pi}{2} = \cos \pi - i \sigma_z \sin \pi = \cos \pi = -1 \quad (5.45)$$

For a spin-1/2 particle, the wavefunction $|\psi\rangle$ changes sign under 2π rotation.

$$R_z(2\pi) = \cos \pi - i \sigma_z \sin \pi = \cos \pi = -1 \quad (5.46)$$

This -1 is the same -1 in \mathcal{T}^2 .

The degeneracy theorem of Kramers

Q: Is $\mathcal{T}^2 = -1$ important?

A: Yes. It has a very important consequence: the degeneracy theorem of Kramers

In a time-reversely invariant system, if $\mathcal{T}^2 = -1$, all the energy levels must be doubly degenerate. In other words, if we have an eigenstate of the Hamiltonian $|\psi\rangle$ with energy E , there must be another state $|\psi'\rangle$ which has the same energy.

- True for a single electron
- True for a system with an odd number of electrons
- True for a system with an odd total number of fermions (electrons, protons, neutrons, etc.)

For a time reversal invariant system, $|\psi\rangle$ and $\mathcal{T}|\psi\rangle$ has the same energy. If we can prove that $|\psi\rangle$ and $\mathcal{T}|\psi\rangle$ are two different quantum states (for $\mathcal{T}^2 = -1$), it proves automatically the theorem of Kramers.

Theorem: if $\mathcal{T}^2 = -1$, $\mathcal{T}|\psi\rangle$ give a quantum state different from $|\psi\rangle$.

Proof: Here we first assume that $\mathcal{T}|\psi\rangle$ give the same quantum state $|\psi\rangle$ and show it leads to contradictions

Assuming $\mathcal{T}|\psi\rangle = e^{i\phi}|\psi\rangle$

$$\mathcal{T}^2|\psi\rangle = \mathcal{T}e^{i\phi}|\psi\rangle = e^{-i\phi}\mathcal{T}|\psi\rangle = e^{-i\phi}e^{i\phi}|\psi\rangle = |\psi\rangle \quad (5.47)$$

$$\mathcal{T}^2 = +1 \quad (5.48)$$

This conclusion is in direct contradiction to the assumption $\mathcal{T}^2 = -1$. Therefore, $\mathcal{T}|\psi\rangle \neq e^{i\phi}|\psi\rangle$ for any quantum state $|\psi\rangle$.

Comment: for $\mathcal{T}^2 = +1$ (integer spin), one can still prove that $|\psi\rangle$ and $\mathcal{T}|\psi\rangle$ have the same energy. However, there, $|\psi\rangle$ and $\mathcal{T}|\psi\rangle$ may be the same state. If they are the same state, we can NOT say that there are two states with the same energy. For example, the ground state of a spinless ($S=0$) particle in a harmonic potential trap. The ground state $|G\rangle$ has $E=\hbar\omega/2$. $\mathcal{T}|G\rangle=|G\rangle$ and $|G\rangle$ is unique and there is no other degenerate state has energy $E=\hbar\omega/2$.

Kramers doublet and time-reversal invariant topological insulators

If we apply the theorem of Kramers to the Bloch wave in an insulator, we found that for any Bloch state $\psi_{n,k,\sigma}$, there is another state $\mathcal{T}\psi_{n,k,\sigma}$ which has the same energy.

$$\mathcal{T}\psi_{n,k,\sigma} = \psi_{n,-k,-\sigma} \quad (5.49)$$

In general, the Kramers doublet are located at different momentum point k and $-k$. However, if $k=0$ or $k=\pi$, $-k$ is just k itself. So we found that at $k=0$ and $k=\pi$, every single energy level is double degenerate.

If we consider mid-gap states near $k=0$ and $k=\pi$, they are strictly degenerate at $k=0$ and $k=\pi$, but the degeneracy is lifted away from these two points (they are known as high symmetry points). Because energy is a smooth function of k , we need to connect these mid gap states at $k=0$ and π . There are two different ways to connect these mid-gap states (see the two figures below).

Case I (figure on the l.h.s.): The two states at $k=0$ are connected to the same Kramers doublet at $k=\pi$.

Case II (figure on the r.h.s.): The two states at $k=0$ are connected to two different Kramers doublets at $k=\pi$ (in an zigzag way).

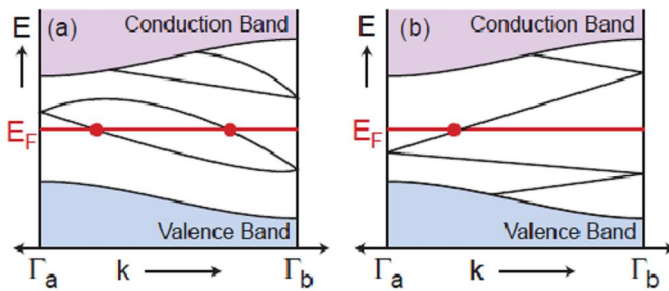


Fig. 1 the edge states

Mid-gap state for a 2D time-reversal invariant topological insulator. (figure from Topological Insulator, by Hasan and Kane, RMP 2011).

For the first case, depending on the chemical potential, we may have no edge states, two pairs of edge states, (or four pairs, or any even numbers). Because this case doesn't always have edge states, they are topologically trivial insulators.

For the second case, no matter what the value of μ is, there are always some edge states. In fact, there are always odd number of left moving edge states and the same number of right moving edge states.

Therefore, we only have two types of insulators in the presence of T-symmetry: (a) trivial insulators which have even pairs of edge states (remember that 0 is an even number) and (b) topological insulators, which have odd pairs of edge states. This is another way to understand why the Z_2 in T-invariant topological insulator.

5.8. 3D topological insulators

Time-reversal invariant topological insulator can be generalized to 3D. 3D topological insulators are described by four Z_2 topological indices. Three of them are known as weak topological indices and the last one is known as the strong topological index.

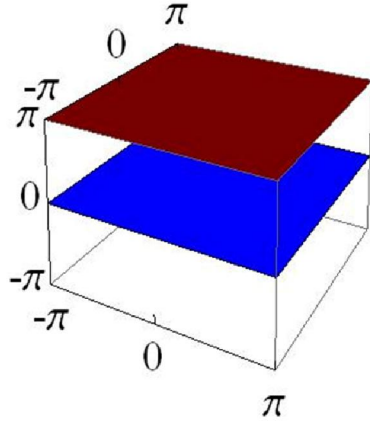


Fig. 2 the BZ of a 3D insulator

Consider the 3D BZ of a 3D insulator. Now, we consider constant k_z planes. We can consider each constant k_z plane as a 2D system. For most constant $-k_z$ planes, they are not time-reversally invariant 2D systems, because $k_z \rightarrow -k_z$ under time-reversal. However, the $k_z = 0$ and $k_z = \pi$ planes are time-reversally invariant, because k_z is the same as $-k_z$ at 0 and π .

Now we consider $k_z = 0$ plane as a 2D time-reversal invariant insulator and $k_z = \pi$ plane as another 2D time-reversal invariant insulator. We can ask whether these two 2D planes are topological insulators or trivial insulators. There are three possibilities: both trivial, both topological, one topological and one trivial.

- Case I: both are trivial: the 3D insulator is topologically trivial
- Case II: both are nontrivial: the 3D insulator is a weak topological insulator.
- Case III: one is trivial and the other is topological: the 3D insulator is a strong topological insulator

Weak topological insulators

For a weak topological insulator, both the $k_z = 0$ and π planes have edge states. Each of them have one pair of edge states as shown in the left figure below. The dots are the Fermi surface for the edge states (where μ crosses with the dispersion relation of the edge states). However, we know that Fermi surfaces are close loops which cannot have starting or ending points. So if we have these six points of Fermi surfaces, we need to connect them to form close loops. So we get the figure on the right.

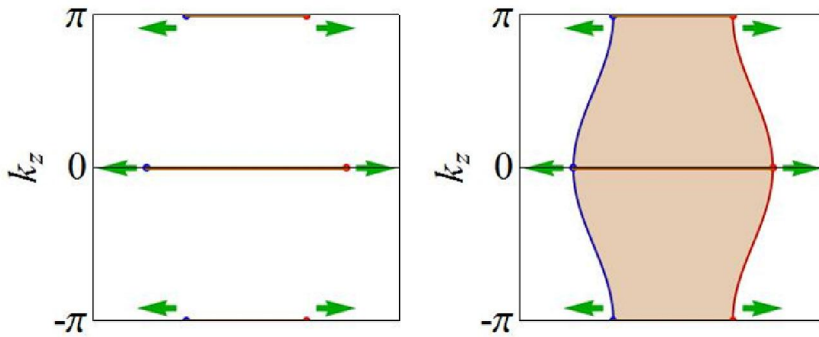


Fig. 3. the surface states of a weak topological insulator

From the figure on the right, we can see that for a 3D weak topological insulator, the 2D surface is a metal, and this surface metal has open Fermi surface as shown in the figure above.

Another way to understand the weak topological insulator is: it is just a stack of 2D topological insulators (stacked along the z-axis).

We can repeat the same argument for constant k_x and k_y planes, which gives us two other types of weak topological insulators. They also correspond to stacks of 2D topological insulators (but are stacked along the x or y axis.)

Strong topological insulators

For a strong topological insulator, only one of the $k_z = 0$ and π planes has edge states (say $k_z = 0$). So we have one pair of edge states as shown in the left figure below. The dots are the Fermi surface for the edge states (where μ crosses with the dispersion relation of the edge states). Again, we know that Fermi surfaces are close loops which cannot have starting or ending points. So if we have these two points of Fermi surfaces, we need to connect them to form close loops. So we get the figure on the right.

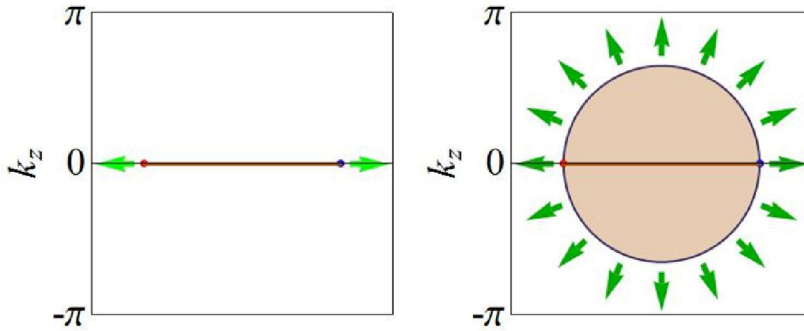


Fig. 4. the surface states of a strong topological insulator

From the figure on the right, we can see that for a 3D strong topological insulator, the 2D surface is a metal, and this surface metal has a closed Fermi surface and the spin rotate by 2π if we goes around the Fermi surface.

We can repeat the same argument for constant k_x and k_y planes. However, they don't give any new information. If we find that the system is a strong topological insulator using constant k_z planes, we will get the same answer using k_x or k_y , so there is just one types of strong topological insulator.

If we change the chemical potential, the Fermi surface changes its size (become bigger or smaller). If the Fermi surface shrink into a point, it is a Dirac point.