5

Topological insulator with time-reversal symmetry

It is impossible to have quantum Hall effect without breaking the time-reversal symmetry. $\mathcal{T}\sigma_{xy} = -\sigma_{xy}$. If we want σ_{xy} to be invariant under $\mathcal{T}$, $\mathcal{T}\sigma_{xy} = \sigma_{xy}$, σ_{xy} must be zero.

Q: Can we have other type of topological insulators, in the presence of $\mathcal{T}$-symmetry? By saying topological insulator, I mean an insulator with a protected metallic edge. By protected, I mean no matter what we do, we cannot turn the metallic edge into an insulating edge.

5.1. spin-orbit coupling

In previous discussions, we ignored the spin degrees of freedom. In reality, we have spin up and spin down electrons. If we consider free electrons moving in 2D (without lattice), the Hamiltonian is:

$$H = \sum_k \frac{k^2}{2m} c_{k\uparrow}^\dagger c_{k\uparrow} + \sum_k \frac{k^2}{2m} c_{k\downarrow}^\dagger c_{k\downarrow} \tag{5.1}$$

Kinetic energy for a particle with momentum k and spin σ, $\epsilon_\sigma(k) = k^2/2m$. The kinetic energy of a particle doesn't depend on the spin degrees of freedom. So we say that: spin degrees of freedom and orbit degrees of freedom (which gives us the kinetic energy) are decoupled.

The Hamiltonian shown above is an idea case. In reality, spin motion and orbit motion are couple together, and extra terms should be added to the Hamiltonian to describe those effect.

More general cases:

Because we have two spin species, the Hamiltonian of the kinetic energy is in general a 2×2 matrix:

$$H = \sum_k \begin{pmatrix} c_{k\uparrow}^\dagger & c_{k\downarrow}^\dagger \end{pmatrix} \mathcal{H} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} \tag{5.2}$$

Because the Hamiltonian is an Hermitian operator, $\mathcal{H}$ must be a Hermitian 2×2 matrix. For any Hermitian 2×2 matrix, we can write it in terms of identity and Pauli matrices.

$$\mathcal{H} = \mathcal{H}_0 I + \mathcal{H}_x \sigma_x + \mathcal{H}_y \sigma_y + \mathcal{H}_z \sigma_z \tag{5.3}$$

(Please notice that we used the similar construction to handle a 2 band system. Although the mathematics are similar, there is one important difference in physics. There for a two-band model, we ignored the spin index and the two-by-two matrix are NOT spin Pauli matrices. They are "pseudo-spins" (to describe the two bands). But here, the Pauli matrices are the true spin Pauli matrices, and they do tell us the spin of an electron.).

For the case we consider above, $\mathcal{H}_x = \mathcal{H}_y = \mathcal{H}_z = 0$, we only have $\mathcal{H}_0 = k^2/2m$. There is no Pauli matrix in the Hamiltonian, which means that the spin degrees of freedom plays no role in the kinetic energy (i.e. spin and orbit motion decouples).

In general, the $\mathcal{H}_x$, $\mathcal{H}_y$, $\mathcal{H}_z$ can be none-zero, so spin plays an role in the kinetic energy.

One example:

$$\mathcal{H}(k) = \begin{pmatrix} \frac{k^2}{2m} + \alpha k & 0 \\ 0 & \frac{k^2}{2m} - \alpha k \end{pmatrix} \tag{5.4}$$

More realistic model:the Rashba spin-orbital coupling:

$$\mathcal{H} = \frac{k^2}{2m} I + \alpha (\sigma \times k)\cdot \hat{z} = \frac{k^2}{2m} I + \alpha \sigma_x k_y - \alpha \sigma_y k_x = \begin{pmatrix} \frac{k^2}{2m} & \alpha k_y + i \alpha k_x \\ \alpha k_y - i \alpha k_x & \frac{k^2}{2m} \end{pmatrix} \tag{5.5}$$

May appear in an anisotropic crystal, the interface between two materials, or the surface of a material. For the interface, because the two materials have different electron density, electron will redistribute near the interface (moving from on material to the other). This induces an E field perpendicular to the interface. Here, the coupling strength α is determined by the strength of this E field

Another example:the Dresselhaus spin-orbital coupling:

$$\mathcal{H}_{\text{Dresselhaus}} = \beta\left[\sigma_x k_x\left(k_y{}^2 - k_z{}^2\right) + \sigma_y k_y\left(k_z{}^2 - k_x{}^2\right) + \sigma_z k_z\left(k_x{}^2 - k_y{}^2\right)\right] \tag{5.6}$$

Time-reversal symmetry

Typically, spin-orbit couplings are described by terms like $\sum_{ij} c_{ij}\, \sigma_i\, k_j{}^{2n+1}$. The spin-orbit coupling PRESERVES the time-reversal symmetry. $\mathcal{T}\sigma \to -\sigma$ and $\mathcal{T}\, k \to -k$

$$\mathcal{T}\, \sigma_i\, k_j{}^{2n+1} = (-\sigma_i)\left(-\, k_j{}^{2n+1}\right) = (-1)^{2n+2}\, \sigma_i\, k_j{}^{2n+1} = \sigma_i\, k_j{}^{2n+1} \tag{5.7}$$

5.2. spin-orbital coupling and magnetic field

Starting from the model we considered above

$$\mathcal{H}(k) = \begin{pmatrix} \frac{k^2}{2m} + \alpha k & 0 \\ 0 & \frac{k^2}{2m} - \alpha k \end{pmatrix} = \begin{pmatrix} \frac{1}{2m}(k^2 + 2\alpha m k + m^2\alpha^2) - m\alpha^2/2 & 0 \\ 0 & \frac{1}{2m}(k^2 - 2\alpha m k + m^2\alpha^2) - m\alpha^2/2 \end{pmatrix} = \begin{pmatrix} \frac{(k+\alpha m)^2}{2m} & 0 \\ 0 & \frac{(k-\alpha m)^2}{2m} \end{pmatrix} - m\alpha^2/2\, I \tag{5.8}$$

Q: What does this Hamiltonian looks like?

A: electrons moving in some magnetic field. But spin up and down electrons feels opposite magnetic field.

$$H = \frac{(k - e\, A)^2}{2m} \tag{5.9}$$

We can see that for spin up electrons, they are coupled to an "magnetic field" with $A_\uparrow = -\alpha m/e$. For spin down electrons, it is coupled to an magnetic field with $A_\downarrow = \alpha m/e$. $A_\uparrow = -A_\downarrow$, so $B_\uparrow = -B_\downarrow$

Notice that this is just a toy model for demonstration purposes. Strictly speaking, one cannot define a vector potential in 1D because B=∇×A, but one cannot define cross product in 1D. So one need a 2D or 3D system to really see the analogy between B field and spin-orbit couplings. And a real system can be much more complicated.

5.3. Topological insulator from spin-orbit effect

- We can get quantum Hall insulators using B field (uniform or staggered)
- Spin-orbit effect is really similar to external B field, $\vec{B}(r)$ for spin up electron and $-\vec{B}(r)$ for spin down electron.

Q: Can we use spin-orbit effect to get topological insulators?

A: Yes. But there are two things different from IQH.

Example: Haldane's model ×2=Kane-Mele Model

- We consider to copies of Haldane's model.
- One for spin up and one for spin down
- The complex hoppings for spin up and down electrons have opposite phase.
  - Spin-up: quantum Hall state with C=1

- Spin-down: quantum Hall state with C=-1
- The whole system still have C=0 (no Hall effect), but this is an insulator with metallic edge states.

Remarks:

- In the model of Haldane, the complex hopping terms was induced by a staggered magnetic field. Here, in the Kane-Melee model, the complex hopping are spin-orbit coupling terms (spin-dependent hopping).
- Seems that the spin-orbit coupling can give us TIs without breaking the time-reversal symmetry.
- But there are two things one needs to notice (which are the key discoveries Kane and Mele made):

Model of Haldane:

$$H = H_{\text{NN}} + H_{\text{NNN}} = \sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} \mathcal{H}_{11}(k) & \mathcal{H}_{12}(k) \\ \mathcal{H}_{21}(k) & \mathcal{H}_{22}(k) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{5.10}$$

$$\mathcal{H}_{12}(k) = -t\left(e^{-i\vec{k}\cdot\vec{e}_1} + e^{-i\vec{k}\cdot\vec{e}_2} + e^{-i\vec{k}\cdot\vec{e}_3}\right) \tag{5.11}$$

$$\mathcal{H}_{21}(k) = \mathcal{H}_{12}(k)^* = -t\left(e^{i\vec{k}\cdot\vec{e}_1} + e^{i\vec{k}\cdot\vec{e}_2} + e^{i\vec{k}\cdot\vec{e}_3}\right) \tag{5.12}$$

$$\mathcal{H}_{11}(k) = -2\,t'\left[\cos(k\cdot v_1 - \phi) + \cos(k\cdot v_2 - \phi) + \cos(k\cdot v_3 - \phi)\right] \tag{5.13}$$

$$\mathcal{H}_{22}(k) = -2\,t'\left[\cos(k\cdot v_1 + \phi) + \cos(k\cdot v_2 + \phi) + \cos(k\cdot v_3 + \phi)\right] \tag{5.14}$$

the Kane-Mele model:

$$H = \sum_k \begin{pmatrix} a_{k\uparrow}^\dagger & b_{k\uparrow}^\dagger & a_{k\downarrow}^\dagger & b_{k\downarrow}^\dagger \end{pmatrix} \begin{pmatrix} \mathcal{H}_{11}(k) & \mathcal{H}_{12}(k) & 0 & 0 \\ \mathcal{H}_{21}(k) & \mathcal{H}_{22}(k) & 0 & 0 \\ 0 & 0 & \mathcal{H}_{11}(k) & \mathcal{H}_{21}(k) \\ 0 & 0 & \mathcal{H}_{12}(k) & \mathcal{H}_{22}(k) \end{pmatrix} \begin{pmatrix} a_{k\uparrow} \\ b_{k\uparrow} \\ a_{k\downarrow} \\ b_{k\downarrow} \end{pmatrix} \tag{5.15}$$

This is an idea model, assuming there is no hybridization between spin up and down electrons (the low-left and upper-right corner of $\mathcal{H}$ are assumed to be zero). But in any real system, this is not the case. One could get extra terms which hybridize the spin up and down electrons (extra terms in the Hamiltonian). In the presence of those extra terms, whether one still have edge states or not is very unclear. By allowing various extra terms in the model, Kane and Mele found:

1. The edge states are only protected in the presence of the time-reversal symmetry. If we break the time-reversal symmetry, the edge state will disappear and the system will turns into a trivial insulator

2. The number of edge states is only well-defined mod 2. So we only have two types of insulators: no edge states (trivial) or 1 pair of edge state (topological). This is very different from IQHE, which can have any number of edge states.

Because we only have 0 or 1 pair of edge states, these insulators are known as Z_2 topological insulators.

5.4. Why Z_2?

Let's check what will happen to the edge states, when we include extra terms into the Hamiltonian.

Case I: 1 pair of edge states.

Let's consider the Kane-Mele model (or any other model with one pair of edge states). Here our spin up electron has C=1, so it has one left moving edge states $\epsilon = v_F\,k$. Spin down electrons have C=-1, so the edge states for spin down electrons are right moving $\epsilon = -v_F\,k$. We can write them together in one Hamiltonian as a 2×2 matrix.

$$\mathcal{H}(k) = \begin{pmatrix} v_F\,k & 0 \\ 0 & -v_F\,k \end{pmatrix} = v_F\,k\,\sigma_z \tag{5.16}$$

Introducing extra terms in the bulk resulting in extra terms in the edge states Hamiltonian.

Q: Can one add any extra term to open a gap for the edge states?

This question is important. If we can open the gap for the edge states, we can move the chemical potential into the gap and the edge states turns into an insulator. If the system have an insulating edge, it is a trivial insulator (edge states are no long topologically protect). But if we can prove that no matter what we do, we can NOT open a gap, the edge is always metallic, so we have a topologically protected edge state (topological insulator).

A: No, if we preserve the time-reversal symmetry. Yes, if we break the time-reversal symmetry. In other words, if the system have time-reversal symmetry, it is a topological states with protected edge states. But if we break the time-reversal symmetry, it is a trivial insulator.

First, let's break the time-reversal symmetry, by adding a $m\,\sigma_z$ term to the Hamiltonian and see what will happen. This term breaks the $\mathcal{T}$-symmetry. $\mathcal{T}\sigma \to -\sigma$. So $\mathcal{T}\; m\,\sigma_z \to -m\,\sigma_z$

$$\mathcal{H}(k) = \begin{pmatrix} v_F\,k & m \\ m & -v_F\,k \end{pmatrix} \tag{5.17}$$

Dispersion:

$$\epsilon_{\pm}(k) = \sqrt{(v_F\,k)^2 + m^2} \tag{5.18}$$

We have a gap in the spectrum of the edge state. The edge state is NOT gapless. If we have chemical potential inside the gap, the edge is NOT a metal. (the system is not a topological insulator).

Second, let's preserve the time-reversal symmetry and see what will happen. If we preserve the time-reversal symmetry, the most general Hamiltonian we can write down is:

$$\mathcal{H}(k) = \sum c_{n,i}\,k^{2n+1}\,\sigma_i + \sum b_n\,k^{2n}\,I \tag{5.19}$$

At $k = 0$,

$$\mathcal{H}(k=0) = b_0\,I = \begin{pmatrix} b_0 & 0 \\ 0 & b_0 \end{pmatrix} \tag{5.20}$$

Eigenvalues at k=0: $\epsilon_{\pm} = b_0$

Gap at k=0: $\Delta(k=0) = \epsilon_+ - \epsilon_- = 0$

No gap! No matter what chemical potential we choose, the system must be a metal at the edge. (a topological insulator).

Case II: 2 pairs of edge states.

Assume the spin up state is in a quantum Hall state with C=2, and the spin down state has C=-2. We will have two left moving electrons with spin up, and two right moving electrons with spin down.

$$H = \sum_k \begin{pmatrix} c_{k\uparrow}^\dagger & d_{k\uparrow}^\dagger & c_{k\downarrow}^\dagger & d_{k\downarrow}^\dagger \end{pmatrix} \mathcal{H} \begin{pmatrix} c_{k\uparrow} \\ d_{k\downarrow} \\ c_{k\downarrow} \\ d_{k\downarrow} \end{pmatrix} \tag{5.21}$$

$$\mathcal{H}(k) = \begin{pmatrix} v_{\mathrm{F}1}\,k & 0 & 0 & 0 \\ 0 & v_{\mathrm{F}2}\,k & 0 & 0 \\ 0 & 0 & -v_{\mathrm{F}1}\,k & 0 \\ 0 & 0 & 0 & -v_{\mathrm{F}2}\,k \end{pmatrix} \tag{5.22}$$

Now, one can add one extra term,

$$\mathcal{H}(k) = \begin{pmatrix} v_{\mathrm{F}1}\,k & 0 & 0 & m \\ 0 & v_{\mathrm{F}2}\,k & -m & 0 \\ 0 & -m & -v_{\mathrm{F}1}\,k & 0 \\ m & 0 & 0 & -v_{\mathrm{F}2}\,k \end{pmatrix} \tag{5.23}$$

This Hamiltonian is time-reversally invairnt. As we will show in the next lecture, the time-reversal operator is

$$U_T = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \tag{5.24}$$

Under time-reversal,

$$\mathcal{H}(k) \to \mathcal{H}'(k) = \left(U_T\,\mathcal{H}(k)\,{U_T}^{-1} \right)^* \tag{5.25}$$

Here * means complex conjugate. It can be easily checked that the $\mathcal{H}$(k) we wrote above is invirant under time-reversal

$$\mathcal{H}(k) \to \mathcal{H}'(k) = \left(U_T \mathcal{H}(k) U_T^{-1} \right)^* = \mathcal{H}(k) \tag{5.26}$$

Here, we consider an simple case with $v_{F1} = v_{F2}$ (for $v_{F1} \neq v_{F2}$, all qualitative results remains the same). The eigenvalues are:

Two degenerate upper band: $\in = \sqrt{m^2 + k^2 v_{F1}^2}$ and two degenerate lower band $\in = -\sqrt{m^2 + k^2 v_{F1}^2}$.

There is a gap Δ=2m.

Generic cases

In a time-reversal invariant 2D system:

- If we have (2n+1) pairs of edge modes, one can add extra terms to gap 2n of them. But there will always be 1 pair which is gapless (topological insulator)
- If we have 2n pairs of edge modes, one can always add some extra term to gap all of them. (trivial insulator)

Connection to high energy, one pair of edge states give us a Weyl fermion. n pairs of edge states gives us n Weyl fermions. If we enforce chiral symmetry, A Weyl fermion can only get mass (open gap) but two Weyl fermion can get mass, by combining them into a Dirac fermion. If we have 2n Weyl fermions, we can pair them up into n Dirac fermions, and give all of them some mass. But if we have 2n+1 Weyl fermions, we cannot do so. We can pair 2n of them into n Dirac fermions and give them mass, but there will be one left, which is massless (i.e. gapless).

5.5. How to compute the topological index for these Z_2 topological insulators.

- More complicated than the Chern number.
- There are many different (but equivalent) ways to do so (in the order of 10).
- Will not be discussed in the lecture because it is too technical (at least to my standard).

Here, I just describe briefly one way to get the topological index:

Step 1, Write down the wavefunction (diagonalize the 2n×2n matrix Hamiltonian for an n-band model).

Step 2, Choose the phase such that $\psi_k = \psi_{-k}^*$, which is always possible because we have the time-reversal symmetry.

Step 3, For a topological insulator, you will find that there is no way to define a wavefunction for every momentum point k. One need to cut the BZ into different regions and use different "gauge" in different regions.

Step 4, the gauge transformation at the boundary defines a winding number (similar to the way we find the Chern number)

Step 5, If the winding number is odd: topological! If it is even, trivial.

Remark: one may choose different gauge to repeat the calculation, and by choosing a different gauge, the winding number one find may change. But the parity of the winding number (even or odd) will never change. This is very different from the quantum Hall, where the winding number is a physical observable and the value has true physical meaning. For T-invariant topological insulators, the winding number is NOT a physical observable, and its value has no physical meaning, BUT, the parity of the winding number is physical and will not change no matter how one do the calculations.

5.6. Comparison between the time-reversal invariant topological insulators (QSHE) and QHE

The time-reversal invariant 2D topological insulators are also known as the quantum spin Hall effect (QSHE).

Symmetry:

- IQHE: Must break the time-reversal symmetry. Otherwise there is no Hall effect.
- QSHE: Must preserve the time-reversal symmetry. Otherwise the edge states are not topologically protected.

Stability:

- IQHE: More stable. Once we have IQHE, as long as we don't close the gap, the edge state will always be there.
- QSHE: Less stable. If one breaks the time-reversal symmetry, the edge states can be killed.

Impurity scatterings

- IQHE: No impurity scatterings at all.
- QSHE: Impurities cannot reflect one electron, because it breaks the time-reversal symmetry. But impurities can reflect two-electrons simultaneously, which doesn't break the time-reversal symmetry. There are impurity scatterings, but it is weaker than an ordinary 1D wire.

Experimental signature:

- IQHE: Quantized Hall conductivity (perfect quantization, error bar 1/10^9).
- QSHE: Conductivity = $2\,e^2/h$ (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 $2\,e^2/h$ 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