$$\mathcal{H}_z = M - 3\sqrt{3}\ t' \sin\phi \tag{3.361}$$

at the K' point

$$\mathcal{H}_z = M + 3\sqrt{3}\ t' \sin\phi \tag{3.362}$$

Therefore, as long as $|M| < |3\sqrt{3}\ t' \sin\phi|$, the system is an topological insulator ($\mathcal{H}_z$ flips sign). If $|M| > |3\sqrt{3}\ t' \sin\phi|$, $\mathcal{H}_z$ is always positive (or negative) and thus the system is topologically trivial.

The marginal case $|M| = |3\sqrt{3}\ t' \sin\phi|$ is a topological transition. Here, $\mathcal{H}_z = 0$ at either the K point or the K' point. Because $\mathcal{H}_x = \mathcal{H}_y = 0$ at these two points, the gap must be zero at one of the two points. So there is a band crossing in the system (either at K o K', depending on the sign of M ant t sin ϕ) and the system is not an insulator.

The insulating gap is closed at the topological transition point.

Remarks:

The model of Haldane is the first example of a topological insulator beyond quantum Hall effect.

It demonstrates that topological insulator is a generic concept, which may appear in any insulating systems (NOT just quantum Hall).

It also demonstrates that as long as the topological index is nonzero, one will observe all the topological phenomena expected for a quantum Hall state, including the quantized Hall conductivity and the existence of the edge states.

The key differences between the model of Haldane and the quantum Hall effects are (1) the B field is on average zero in the model of Haldane while the QHE has a uniform B field and (2) there is a very strong lattice background in the model of Haldane while the QHE requires weak lattice potential.

Systems similar to the Haldane's model are known as topological Chern insulators or Chern insulators (average B is 0 and have a strong lattice potential). But sometimes, Chern insulator are also used to refer to the quantum Hall effect.

The model of Haldane is also the foundation to explore more complicated and exotic topological states. For example, the time-reversal invariant topological insulators was first proposed using a modified Haldane's models, which we will study latter in the semester.

3.15. Some symmetry properties of the Berry curvature $\mathcal{F}$ and the Chern number.

3.15.1. time-reversal transformation $\mathcal{T}$ and time-reversal symmetry

In this section, we consider systems with time-reversal symmetry and shows that in the presence of the time-reversal symmetry, the Chern number must be zero. Therefore, to get a topological insulator with nonzero C, one must break the time-reversal symmetry.

Dispersion relation

Dispersion relation under time-reversal transformation:

$$\mathcal{T}\,\epsilon_n(k) = \epsilon_n(-k) \tag{3.363}$$

This is because $\mathcal{T}$ turns $\vec{k}$ into $-\vec{k}$.

There are two ways to see that $\mathcal{T}$ turns $\vec{k}$ into $-\vec{k}$.

- $\vec{k}$ is the momentum of a state. Under time-reversal, velocity changes sign, so does the momentum.
- $\vec{k} = -i\,\partial_r$. Under $\mathcal{T}$, ∂_r remains invariant. However, because $\mathcal{T}$ is an anti-unitary transformation (which changes a complex number to its complex conjugate), it flips the sign of i. Therefore, $\mathcal{T}\,\vec{k} = \mathcal{T}(-i\,\partial_r) = i\,\partial_r = -\vec{k}$.

If the system is time-reversally invariant, the time-reversal symmetry implies that $\epsilon_n(k)$ is invariant under time-reversal transformation

$$\mathcal{T}\,\epsilon_n(k) = \epsilon_n(k) \tag{3.364}$$

Compare the two equations, we have:

$$\epsilon_n(k) = \epsilon_n(-k) \tag{3.365}$$

Bottom line: For systems with time-reversal symmetry, the dispersion is an even function of the momentum $\vec{k}$.

Bloch wave function $\psi_{n,k}(r) = u_{n,k}(r)\, e^{i k r}$

Bloch wave under time-reversal transformation:

$$\mathcal{T}\, u_{n,k}(r) = u_{n,-k}(r)^* \tag{3.366}$$

Here, $\mathcal{T}$ changes k to $-k$ (same as the dispersion relation). In addition, because $u_{n,k}(r)$ is in general a complex function, $\mathcal{T}$ changes the function to its complex conjugate.

If the system is time-reversally invariant,

$$\mathcal{T}\, u_{n,k}(r) = e^{i\,\phi(k)}\, u_{n,k}(r) \tag{3.367}$$

By comparing the two equations above, we found that for a system with time-reversal symmetry,

$$u_{n,-k}(r)^* = e^{i\,\phi(k)}\, u_{n,k}(r) \tag{3.368}$$

This arbitrary phase is here because wavefunctions are defined up to an arbitrary phase

Berry connection $\mathcal{A}_n(k) = -i\,\langle u_{n,k} \mid \nabla_k \mid u_{n,k}\rangle$

The Berry connection is defined as:

$$\mathcal{A}_n(k) = -i\,\langle u_{n,k} \mid \nabla_k \mid u_{n,k}\rangle = -i \int d\vec{r}\; u_{n,k}(\vec{r})^*\, \partial_k\, u_{n,k}(\vec{r}) \tag{3.369}$$

The under time-reversal, the new $\mathcal{A}_n(k)$ is defined as

$$\begin{aligned}\mathcal{T}\mathcal{A}_n(k) &= -i\,\langle \mathcal{T}\, u_{n,k} \mid \nabla_k \mid \mathcal{T}\, u_{n,k}\rangle = -i \int d\vec{r}\; u_{n,-k}(\vec{r})\, \partial_k\, u_{n,-k}(\vec{r})^* = \\ &i \int d\vec{r}\; \partial_k\, u_{n,-k}(\vec{r})\, u_{n,-k}(\vec{r})^* = -i \int d\vec{r}\; u_{n,-k}(\vec{r})^*\, \partial_{-k}\, u_{n,-k}(\vec{r}) = -i\,\langle u_{n,-k} \mid \nabla_{-k} \mid u_{n,-k}\rangle = \mathcal{A}_n(-k)\end{aligned} \tag{3.370}$$

If the system has time-reversal symmetry

$$\mathcal{T}\mathcal{A}_n(k) = \mathcal{A}_n(k) + \nabla_k\, \chi(k) \tag{3.371}$$

So we have

$$\mathcal{A}_n(-k) = \mathcal{A}_n(k) + \nabla_k\, \chi(k) \tag{3.372}$$

Bottom line: For systems with time-reversal symmetry, $\mathcal{A}_n(-k)$ and $\mathcal{A}_n(k)$ differs by a gauge transformation $\nabla_k\, \chi(k)$.

Berry curvature $\mathcal{F}_n(k) = -i\epsilon_{ij}\,\langle \partial_i\, u_{n,k} \mid \partial_j\, u_{n,k}\rangle$

The Berry curvature is defined as:

$$\mathcal{F}_n(k) = -i\epsilon_{ij}\,\langle \partial_{ki}\, u_{n,k} \mid \partial_{kj}\, u_{n,k}\rangle = -i\,\epsilon_{ij} \int d\vec{r}\; \partial_{ki}\, u_{n,k}(\vec{r})^*\, \partial_{kj}\, u_{n,k}(\vec{r}) \tag{3.373}$$

The under time-reversal, the new $\mathcal{F}_n(k)$ is defined as

$$\begin{aligned}\mathcal{T}\mathcal{F}_n(k) &= -i\epsilon_{ij}\,\langle \partial_{ki}\,\mathcal{T}u_{n,k} \mid \partial_{kj}\,\mathcal{T}u_{n,k}\rangle = \\ &-i\,\epsilon_{ij} \int d\vec{r}\; \partial_{ki}\,\mathcal{T}u_{n,k}(\vec{r})^*\, \partial_{kj}\,\mathcal{T}u_{n,k}(\vec{r}) = -i\,\epsilon_{ij} \int d\vec{r}\; \partial_{ki}\, u_{n,-k}(\vec{r})\, \partial_{kj}\, u_{n,-k}(\vec{r})^* = -i\,\epsilon_{ij} \int d\vec{r}\; \partial_{kj}\, u_{n,-k}(\vec{r})^*\, \partial_{ki}\, u_{n,-k}(\vec{r})\end{aligned} \tag{3.374}$$

If we swap i and j here

$$\mathcal{T}\mathcal{F}_n(k) = -i\,\epsilon_{ji} \int d\vec{r}\; \partial_{ki}\, u_{n,-k}(\vec{r})^*\, \partial_{kj}\, u_{n,-k}(\vec{r}) = i\,\epsilon_{ij} \int d\vec{r}\; \partial_{ki}\, u_{n,-k}(\vec{r})^*\, \partial_{kj}\, u_{n,-k}(\vec{r}) = -\mathcal{F}_n(-k) \tag{3.375}$$

If the system has time-reversal symmetry

$$\mathcal{T}\mathcal{F}_n(k) = \mathcal{F}_n(k) \tag{3.376}$$

So we have

$$\mathcal{F}_n(-k) = -\mathcal{F}_n(k) \tag{3.377}$$

Bottom line: For systems with time-reversal symmetry, $\mathcal{F}_n(k)$ is an odd function of k

A direct result: Because the integral of an odd function over the whole Brillouin zone must be zero, (the contribution from k and -k cancels each other), the Chern number for a time-reversally invariant system must be C=0.

The Chern number C = $\frac{1}{2\pi}\iint d\,k \mathcal{F}_n(\mathbf{k})$

$$\mathcal{T}C = \mathcal{T}\frac{1}{2\pi}\iint d\,k_x\,d\,k_y\,\mathcal{F}_n(k) = -\frac{1}{2\pi}\iint d\,k_x\,d\,k_y\,\mathcal{F}_n(-k) = -\frac{1}{2\pi}\iint d\,k_x\,d\,k_y\,\mathcal{F}_n(k) = -C \tag{3.378}$$

If the system has time-reversal symmetry,

$$\mathcal{T}C = C, \tag{3.379}$$

So we have C=-C, which means C=0.

Bottom line: to have a nontrivial Chern number, the system must break the time-reversal symmetry (using external B field or some other method).

3.15.2. Space-inversion transformation $\mathcal{I}$ and space-inversion symmetry

Space inversion transformation $\mathcal{I}$ turns a vector $\vec{r}$ into $-\vec{r}$. It also changes $\vec{k}$ into $-\vec{k}$, which is similar to $\mathcal{T}$. However, $\mathcal{I}$ is an unitary transformation, while $\mathcal{T}$ is anti-unitary.

Dispersion relation

Dispersion relation under time-reversal transformation:

$$\mathcal{I}\epsilon_n(k) = \epsilon_n(-k) \tag{3.380}$$

If the system is invariant under space inversion

$$\mathcal{I}\,\epsilon_n(k) = \epsilon_n(k) \tag{3.381}$$

Compare the two equations, we have:

$$\epsilon_n(k) = \epsilon_n(-k) \tag{3.382}$$

Bottom line: For systems invariant under space inversion, the dispersion is an even function of the momentum $\vec{k}$.

If one want make a system where the dispersion is NOT an even function, one need to break both space inversion symmetry and time-reversal symmetry.

Bloch wave function $\psi_{n,k}(\mathbf{r}) = u_{n,k}(\mathbf{r})\,e^{i\,k\,r}$

$$\mathcal{I}\,u_{n,k}(r) = u_{n,-k}(r) \tag{3.383}$$

If the system is invariant under space inversion

$$\mathcal{I}\,u_{n,k}(r) = e^{i\,\phi(k)}\,u_{n,k}(r) \tag{3.384}$$

By comparing the two equations above, we found that for a system with time-reversal symmetry,

$$u_{n,-k}(r) = e^{i\,\phi(k)}\,u_{n,k}(r) \tag{3.385}$$

Berry connection $\mathcal{A}_n(\mathbf{k}) = -i\langle u_{n,k} \mid \nabla_k \mid u_{n,k}\rangle$

$$\mathcal{I}\mathcal{A}_n(k) = \mathcal{A}_n(-k) \tag{3.386}$$

If the system is invariant under space inversion

$$\mathcal{I}\mathcal{A}_n(k) = \mathcal{A}_n(k) + \nabla_k\,\chi(k) \tag{3.387}$$

So we have

$$\mathcal{A}_n(-k) = \mathcal{A}_n(k) + \nabla_k\,\chi(k) \tag{3.388}$$

Bottom line: For systems invariant under space inversion, $\mathcal{A}_n(-k)$ and $\mathcal{A}_n(k)$ differs by a gauge transformation $\nabla_k\,\chi(k)$.

Berry curvature $\mathcal{F}_n(\mathbf{k}) = -i\epsilon_{ij}\langle\partial_i u_{n,k} \mid \partial_j u_{n,k}\rangle$

$$\mathcal{I}\mathcal{F}_n(k) = \mathcal{F}_n(-k) \tag{3.389}$$

If the system is invariant under space inversion

$$\mathcal{I}\mathcal{F}_n(k) = \mathcal{F}_n(k) \tag{3.390}$$

So we have

$$\mathcal{F}_n(-k) = \mathcal{F}_n(k) \tag{3.391}$$

Bottom line: For systems invariant under space inversion, $\mathcal{F}_n(k)$ is an even function of k

Time-reversal symmetry tell us $\mathcal{F}_n(k)$ is an odd function of k. If system have both $\mathcal{T}$ and $\mathcal{I}$ symmetry, $\mathcal{F}$ must be both an even function and an odd function. So $\mathcal{F}$=0 at any k point.

The Chern number C = $\frac{1}{2\pi}\iint d\,k\mathcal{F}_n(k)$

$$\mathcal{I}C = C \tag{3.392}$$

3.15.3. $\mathcal{I}\,\mathcal{T}$ transformation and $\mathcal{I}\mathcal{T}$ symmetry

Under $\mathcal{I}\mathcal{T}$,

$$\mathcal{I}\mathcal{T}\mathcal{F}_n(k) = \mathcal{I}[-\mathcal{F}_n(-k)] = -\mathcal{F}_n(k) \tag{3.393}$$

If system is invariant under $\mathcal{I}\mathcal{T}$,

$$\mathcal{I}\mathcal{T}\mathcal{F}_n(k) = -\mathcal{F}_n(k) \tag{3.394}$$

So, we have

$$\mathcal{F}_n(k) = -\mathcal{F}_n(k) \tag{3.395}$$

Bottom line: For systems invariant under $\mathcal{I}\mathcal{T}$, $\mathcal{F}_n(k) = 0$ at every k.

For $\mathcal{T}$ symmetry, the integral of $\mathcal{F}$ is zero (C=0), but $\mathcal{F}$ can be nonzero at each k point.

For $\mathcal{I}\mathcal{T}$ symmetry, $\mathcal{F}$ is zero at every single k point. This is a stronger statement!

But there are exceptions. For systems with $\mathcal{I}\mathcal{T}$ symmetry, $\mathcal{F}$ can actually be nonzero.

3.16. π flux and Dirac points

3.16.1. magnetic field, Aharonov–Bohm effect and magnetic π- flux

Q: Why B changes sign under $\mathcal{T}$?

A: Many ways to see it. Here, I use the A-B effect.

In the presence of B field, Aharonov and Bohm tells us that if we move a charged-particle around a closed loop, the electron will pick up a phase, and the phase is the total magnetic field enclosed by the loop (times e/ℏ)

$$\phi = e/\hbar \iint B \cdot d\,S = e/\hbar \oint A.d\,l \tag{3.396}$$

Under time-reversal $e^{i\phi}$ turns into $e^{-i\phi}$, because time-reversal is anti-unitary. So the A-B phase changes sign

$$\mathcal{T}\phi = -\phi \tag{3.397}$$

In other words, the integral of B changes sign

$$\mathcal{T}\iint_D B \cdot d\,S = -\iint_D B \cdot d\,S \tag{3.398}$$

Because this equation is true for any region D, we have $B = -B$.

If a system has time-reversal symmetry, everything must remain the same before and after we flip the arrow of time, including the A-B phase

$$e^{i\phi} = e^{-i\phi} \tag{3.399}$$

Therefore, we have $\phi = -\phi$. So we have ϕ=0 for any region D, which implies that $B = 0$.

Q: Do we really need to have $B = 0$ to preserve the time-reversal symmetry.

A: NO!

This is because a phase is only well-define up to mod 2π. The time-reversal symmetry requires $e^{i\phi} = e^{-i\phi}$, which does NOT implies $\phi = -\phi$. In fact, as long as $\phi = -\phi + 2\,n\,\pi$, the A-B phase will be the same before and after the time-reversal transformation.

This means that to preserve the time-reversal symmetry we just need $\phi = n\,\pi$ while n don't need to be 0.

So we need to have $\int\int_D B \cdot d\,S = n\,\pi$ for any D. This means that B can contains some delta functions.

$$B = \frac{\hbar}{e} \sum_i n_i\,\pi\,\delta(r - r_i) \tag{3.400}$$

For this B field, the integral of B in region D is just

$$\phi = e/\hbar \int\int B \cdot d\,S = \left(\sum_i{}' n_i\right)\pi \tag{3.401}$$

Here the sum $\sum_i{}'$ is over all r_i inside D. A delta function in B is a magnetic flux, which is known as a n×π-flux. These flux doesn't break the time-reversal symmetry.

In addition, it worthwhile to point out that for the A-B phase is only well defined up to mod 2π. So all the 2nπ fluxes give the same A-B phase, which is 0. All the (2n+1)π fluxes give the same A-B phase, which is π.

3.16.2. Berry flux

We can do the same thing for the Berry curvature $\mathcal{F}$(k). If we goes around a contour in the k-space, the phase change of the Bloch wave function around this contour is

$$\phi = \int\int_D \mathcal{F}\,d\,k^2 \tag{3.402}$$

This is known as the Berry phase.

Under $\mathcal{I}\mathcal{T}$, D is invariant so

$$\mathcal{I}\mathcal{T}\,\phi = \mathcal{I}\mathcal{T} \int\int_D \mathcal{F}(k)\,d\,k^2 = -\int\int_D \mathcal{F}(k)\,d\,k^2 = -\phi \tag{3.403}$$

If the system is $\mathcal{I}\mathcal{T}$ invariant, we must have ϕ=-ϕ (but up to mod 2π).

$$\phi = -\phi + 2\,n\,\pi \tag{3.404}$$

so

$$\phi = n\,\pi \tag{3.405}$$

As a result, if we have $\mathcal{I}\mathcal{T}$ symmetry, $\int\int_D \mathcal{F}\,d\,k^2$=n$\pi$ for any region D. So $\mathcal{F}$ must be either 0 or some delta functions.

$$\mathcal{F}(k) = \sum_i n_i\,\pi\,\delta(k - k_i) \tag{3.406}$$

These delta functions are known as Berry fluxes. Because the Berry phase is only well defined up to mod 2π, we have in general two types of Berry fluxes: 0 and π. And a π flux is a Dirac point.

3.16.3. Dirac point

Near a Dirac point, the kernel of the Hamiltonian is:

$$\mathcal{H} = v_F \begin{pmatrix} 0 & \text{kx} - i\,\text{ky} \\ \text{kx} + i\,\text{ky} & 0 \end{pmatrix} \tag{3.407}$$

Using polar coordinates

$$\mathcal{H} = v_F\,k \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \tag{3.408}$$

The eigenvalues for this matrix is $\epsilon_\pm = \pm v_F\,k$. The eigenvectors are:

$$u_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix} \text{ and } u_- = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-i\phi} \\ 1 \end{pmatrix} \tag{3.409}$$

The Berry connection in the polar coordinates has two components, radius and angle.

$$A_{+k} = -i \langle u_+ \mid \partial_k \mid u_+ \rangle = 0 \tag{3.410}$$

$$A_{+\phi} = -\frac{i}{k} \langle u_+ \mid \partial_\phi \mid u_+ \rangle = -\frac{i}{k} \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{i\phi} & 1 \end{pmatrix} \partial_\phi \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-i\phi} \\ 1 \end{pmatrix} = -\frac{i}{k} \frac{1}{2} \begin{pmatrix} e^{i\phi} & 1 \end{pmatrix} \begin{pmatrix} -i\, e^{-i\phi} \\ 1 \end{pmatrix} = -\frac{1}{2k} \tag{3.411}$$

Let's choose a small circle around the Dirac point, the flux through this circle is:

$$\chi = \int\int \mathcal{F}\, dk = \oint \mathcal{A} \cdot dk = \int_0^{2\pi} \mathcal{A}_\phi\, k\, d\phi = -\int_0^{2\pi} \frac{1}{2k} k\, d\phi = -\frac{1}{2} \int_0^{2\pi} d\phi = -\pi \tag{3.412}$$

3.16.4. Why Dirac point is so stable?

This is because the Berry fluxes are very stable. If one has $\mathcal{TI}$ symmetry, the Berry curvature must be

$$\mathcal{F}(k) = \sum_i n_i\, \pi\, \delta(k - k_i) \tag{3.413}$$

Now, if we continuously tune some control parameter in our system, $\mathcal{F}$(k) must change continuously. However, if we have $\mathcal{TI}$ symmetry, the form of $\mathcal{F}$ cannot change, the only thing that can change continuously is the location of the delta functions.

In other words, without break the $\mathcal{TI}$ symmetry, one can only move the Dirac points around in the k-space. They cannot disappear. (However, two Dirac points can annihilate each other).