- Using these $u_{n,\alpha}(k)$, we can define the Berry connection, Berry curvature and the Chern number. Just replace the integral in the real space by summing over i=1…n

Before 80s, people will just stop at step #3, without calculating the eigenvectors. This is because eigenvectors are the wavefunction, which cannot be measured directly in experiments. So people only care about the eigenvalues, which is the dispersion relation (a physical observable).

After the discovery of topological insulators, physicists realized that although the wavefunction can not be measured directly, it contains the topological information, which is a physical observable (the Hall conductivity).

3.13. Example: a topologically-nontrival model

Example:

$$\mathcal{H} = \begin{pmatrix} -2\,t\cos k_x - 2\,t\cos k_y - \mu & \Delta\left(\sin k_x - i\sin k_y\right) \\ \Delta\left(\sin k_x + i\sin k_y\right) & 2\,t\cos k_x + 2\,t\cos k_y + \mu \end{pmatrix} \tag{3.258}$$

Here, we assume $\Delta>0$ and $t>0$ and $-4|t|<\mu<4|t|$.

This is the Hamiltonian of a p+i p superconductor, which will be discussed later. Although it is not the Hamiltonian of an insulator, the physics are essentially the same.

Here, I will not discuss about where this Hamiltonian comes from. We just use it as an example to demonstrate the nontrivial topological index. Let's assume that in some tight-binding model, we get a kernal of the Hamiltonian like this.

Here I use μ to refer to some control parameter, which is NOT the chemical potential.

3.13.1. More general case

For any two-band models, $\mathcal{H}$ is a two-by-two Hermitian matrix.

For a two-by-two Hermitian matrix, one can always separate it into I, and σ_i

$$\mathcal{H} = \mathcal{H}_0(k)\, I + \mathcal{H}_x(k)\,\sigma_x + \mathcal{H}_y(k)\,\sigma_y + \mathcal{H}_z(k)\,\sigma_z \tag{3.259}$$

$\mathcal{H}_0(k)$, $\mathcal{H}_x(k)$, $\mathcal{H}_y(k)$ and $\mathcal{H}_z(k)$ are real functions of k. If we define $\vec{\mathcal{H}}(k) = \left(\mathcal{H}_x(k),\ \mathcal{H}_y(k),\ \mathcal{H}_z(k)\right)$,

$$\mathcal{H} = \mathcal{H}_0(k)\, I + \vec{\mathcal{H}}(k)\cdot\vec{\sigma} \tag{3.260}$$

This is rather similar to a spin S=1/2 in a magnetic field.

$$H = \text{constant} + \mu\,\vec{B}\cdot\vec{\sigma} \tag{3.261}$$

For the case studied here,

$$\mathcal{H}_0(k) = 0 \tag{3.262}$$

$$\mathcal{H}_x(k) = \Delta\sin(k_x) \tag{3.263}$$

$$\mathcal{H}_y(k) = \Delta\sin\left(k_y\right) \tag{3.264}$$

$$\mathcal{H}_z(k) = -2\,t\cos k_x - 2\,t\cos k_y - \mu \tag{3.265}$$

The eigenvalues of $\mathcal{H}$ are

$$E_\pm = \mathcal{H}_0(k) \pm \left|\vec{\mathcal{H}}(k)\right| = \mathcal{H}_0(k) \pm \sqrt{\mathcal{H}_x(k)^2 + \mathcal{H}_y(k)^2 + \mathcal{H}_z(k)^2} \tag{3.266}$$

Pretty much the same as the spin case, where

$$E = \text{constant} + \mu\left|\vec{B}\right| \tag{3.267}$$

For the top band, $E_+ \geq \mathcal{H}_0$, for the lower band $E_- \leq \mathcal{H}_0$. The energy gap is:

$$\Delta(k) = E_+(k) - E_-(k) = 2\left|\vec{\mathcal{H}}(k)\right| \tag{3.268}$$

As long as $\vec{\mathcal{H}}(k) \neq 0$, the two band will not cross with each other.

Let's focus on the lower band (E_-), its eigenvector is

$$u^{(I)}{}_-(k) = \frac{1}{\mathcal{N}^{(I)}}\begin{pmatrix} \mathcal{H}_z(k) - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\,\mathcal{H}_y(k) \end{pmatrix} \tag{3.269}$$

This wavefunction is singular if $\mathcal{H}_x(k) = \mathcal{H}_y(k) = 0$ and $\mathcal{H}_z > 0$,

$$u^{(I)}{}_-(k) = \frac{1}{\mathcal{N}^{(I)}}\begin{pmatrix} \mathcal{H}_z - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\,\mathcal{H}_y(k) \end{pmatrix} = \frac{1}{\mathcal{N}^{(I)}}\begin{pmatrix} \mathcal{H}_z - \sqrt{\mathcal{H}_z(k)^2} \\ 0 \end{pmatrix} = \frac{1}{\mathcal{N}^{(I)}}\begin{pmatrix} \mathcal{H}_z - |\,\mathcal{H}_z(k)\,| \\ 0 \end{pmatrix} = \frac{1}{\mathcal{N}^{(I)}}\begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{3.270}$$

This is indeed a problem for the Hamiltonian shown above. At $k_x = k_y = \pi$.

$$\mathcal{H}_0(k) = 0 \tag{3.271}$$

$$\mathcal{H}_x(k) = \Delta \sin(k_x) = 0 \tag{3.272}$$

$$\mathcal{H}_y(k) = \Delta \sin\left(k_y\right) = 0 \tag{3.273}$$

$$\mathcal{H}_z(k) = -2\,t\cos k_x - 2\,t\cos k_y - \mu = 4\,t - \mu > 0 \tag{3.274}$$

In fact, there is another way to write down the same eigenvector (a phase shift)

$$u^{(\mathrm{II})}{}_-(k) = \frac{1}{\mathcal{N}^{(I)}}\begin{pmatrix} \mathcal{H}_z - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\,\mathcal{H}_y(k) \end{pmatrix} \times \frac{\frac{\mathcal{H}_z + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\,\mathcal{H}_y(k)}}{\left|\frac{\mathcal{H}_z + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\,\mathcal{H}_y(k)}\right|} = \frac{1}{\mathcal{N}^{(\mathrm{II})}}\begin{pmatrix} \frac{-\mathcal{H}_x(k)^2 - \mathcal{H}_y(k)^2}{\mathcal{H}_x(k) + i\,\mathcal{H}_y(k)} \\ \mathcal{H}_z + \left|\vec{\mathcal{H}}(k)\right| \end{pmatrix} = \frac{1}{\mathcal{N}^{(\mathrm{II})}}\begin{pmatrix} -\mathcal{H}_x(k) + i\,\mathcal{H}_y(k) \\ \mathcal{H}_z + \left|\vec{\mathcal{H}}(k)\right| \end{pmatrix} \tag{3.275}$$

$$u^{(\mathrm{II})}{}_-(k) = u^{(I)}{}_-(k)\, e^{i\,\phi(k)} \tag{3.276}$$

This new wavefunction is well defined at $\mathcal{H}_x(k) = \mathcal{H}_y(k) = 0$ and $\mathcal{H}_z(k) > 0$. However, it is NOT well defined at $\mathcal{H}_x(k) = \mathcal{H}_y(k) = 0$ and $\mathcal{H}_z(k) < 0$,

$$u^{(\mathrm{II})}{}_-(k) = \frac{1}{\mathcal{N}^{(\mathrm{II})}}\begin{pmatrix} -\mathcal{H}_x(k) + i\,\mathcal{H}_y(k) \\ \mathcal{H}_z(k) + \left|\vec{\mathcal{H}}(k)\right| \end{pmatrix} = \frac{1}{\mathcal{N}^{(\mathrm{II})}}\begin{pmatrix} 0 \\ \mathcal{H}_z(k) + \sqrt{\mathcal{H}_z(k)^2} \end{pmatrix} = \frac{1}{\mathcal{N}^{(\mathrm{II})}}\begin{pmatrix} 0 \\ \mathcal{H}_z(k) + |\,\mathcal{H}_z(k)\,| \end{pmatrix} = \frac{1}{\mathcal{N}^{(\mathrm{II})}}\begin{pmatrix} 0 \\ \mathcal{H}_z(k) - \mathcal{H}_z(k) \end{pmatrix} = 0 \tag{3.277}$$

For the Hamiltonian shown above, the origin is such a point. $k_x = k_y = 0$

$$\mathcal{H}_0(k) = 0 \tag{3.278}$$

$$\mathcal{H}_x(k) = \Delta \sin(k_x) = 0 \tag{3.279}$$

$$\mathcal{H}_y(k) = \Delta \sin\left(k_y\right) = 0 \tag{3.280}$$

$$\mathcal{H}_z(k) = -2\,t\cos k_x - 2\,t\cos k_y - \mu = -4\,t - \mu < 0 \tag{3.281}$$

Therefore, we need to cut the BZ into two areas and use two different wave functions to describe the Bloch waves. They are connected by a gauge transformation

$$u^{(\mathrm{II})}{}_-(k) = u^{(I)}{}_-(k)\, e^{i\,\phi(k)} \tag{3.282}$$

$$\mathcal{A}_-{}^{(\mathrm{II})}(k) = \mathcal{A}_-{}^{(I)}(k) + \nabla_k\,\phi(k) \tag{3.283}$$

This is in strong analogy to the magnetic monopole case.

Some comments:

- These singularities are NOT physical. If one measure any physical observables, there is no singularity anywhere in the momentum space. However. for the wavefunction and the Berry connection, which are not physical observables, there is always some singularity for this Hamiltonian.
- The location of these singularity points depends on the gauge (phase) choice. In other words, the location of the singularities has no physical meaning either.

- Only one thing about these singularities are physical. That is: there must be some singularity points. This statement is independent of gauge choice and it tells us that the topological index is nonzero.

Let's compute the topological index for this model. For these model, there are four special points which satisfy $\mathcal{H}_x = \mathcal{H}_y = 0$. They are $\vec{k} = (0, 0)$, $\vec{k} = (\pi, \pi)$, $\vec{k} = (0, \pi)$ and $\vec{k} = (\pi, 0)$

At these four points, the values of $\mathcal{H}_z$ are: $\mathcal{H}_z = -4\,t - \mu$, $4\,t - \mu$, $-\mu$ and $-\mu$ respectively.

3.13.2. case I: $\mu < -4\,t$

If $\mu < -4\,t$, all the four special points has $\mathcal{H}_z > 0$. So we can use $u^{(\mathrm{II})}\_(k)$ for the whole BZ, and there is no singularity points.

$$u^{(\mathrm{II})}\_(k) = \frac{1}{\mathcal{N}^{(I)}} \begin{pmatrix} \mathcal{H}_z(k) - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\,\mathcal{H}_y(k) \end{pmatrix} \tag{3.284}$$

Then we can get Berry connection

$$\mathcal{A}\_^{(\mathrm{II})} = -i\,\langle u\_(k) \,|\, \partial_k \,|\, u\_(k)\rangle = -i\left[u^{(\mathrm{II})}\_(k)\right]^\dagger \partial_k\, u^{(\mathrm{II})}\_(k) = -i\sum\nolimits_{\alpha=1}^{2} u^{(\mathrm{II})}\_{,\alpha}(k)^*\, \partial_k\, u\_{,\alpha}(k) \tag{3.285}$$

where $\left[u^{(I)}\_(k)\right]^\dagger$ is the Hermitian conjugate of $u^{(I)}\_(k)$, i.e. complex conjugate and transpose. $\left[u^{(I)}\_(k)\right]^\dagger$ is a row vector, while $u^{(I)}\_(k)$ is a column vector.

The Berry curvature:

$$\Omega\_ = \nabla \times \mathcal{A}\_ \tag{3.286}$$

The total Berry curvature (2π times the Chern number)

$$\iint_{\mathrm{BZ}} d\!k\, \Omega\_ = \iint_{\mathrm{BZ}} d\!k\, \nabla \times \mathcal{A}\_ = \oint_{\partial \mathrm{BZ}} d\!k\, \mathcal{A}\_ = 0 \tag{3.287}$$

The Chern number:

$$C = \frac{1}{2\,\pi} \iint_{\mathrm{BZ}} d\!k\, \Omega\_ = 0. \tag{3.288}$$

3.13.3. Marginal case: $\mu = -4\,t$

$\mathcal{H}_x(k) = \mathcal{H}_y(k) = \mathcal{H}_z(k) = 0$ at k=(π,π)

Because the gap between the two bands is

$$\Delta(k) = E_+ - E\_ = 2\left|\vec{\mathcal{H}}(k)\right| \tag{3.289}$$

$\Delta(k) = 0$ at k=(π,π).

The gap closes at k=(π,π), i.e. the two energy bands touch each other at k=(π,π). This gives us a Dirac point.

Not an insulator (no gap). So we cannot define a topological index.

3.13.4. case II: $-4\,t < \mu < 0$

For $-4\,t < \mu < 0$, $\mathcal{H}_z < 0$ at k=(0,0), and $\mathcal{H}_z > 0$ for all three other points.

Therefore, we need two wave-functions.

Near k=(0,0), we use

$$u^{(I)}\_(k) = \frac{1}{\mathcal{N}^{(I)}} \begin{pmatrix} \mathcal{H}_z(k) - \left|\vec{\mathcal{H}}(k)\right| \\ \mathcal{H}_x(k) + i\,\mathcal{H}_y(k) \end{pmatrix} \tag{3.290}$$

Near the other three special points, we use

$$u^{(\mathrm{II})}{}_{-}(k)=\frac{1}{\mathcal{N}^{(I)}}\begin{pmatrix}\mathcal{H}_z(k)-\left|\vec{\mathcal{H}}(k)\right|\\ \mathcal{H}_x(k)+i\,\mathcal{H}_y(k)\end{pmatrix} \tag{3.291}$$

We can cut the BZ into two parts using a circle around the origin. In side the circle, D_I, we use $u^{(I)}$. Outside the circle we use $u^{(\mathrm{II})}$. This will give as two different Berry connections. In region D^I, we have $A^{(I)}$, and in region D_{II} we have $A^{(\mathrm{II})}$. The are connected by a gauge transformation:

$$u^{(\mathrm{II})}{}_{-}(k)=u^{(I)}{}_{-}(k)\,e^{i\,\phi(k)} \tag{3.292}$$

$$\mathcal{A}_{-}{}^{(\mathrm{II})}(k)=\mathcal{A}_{-}{}^{(I)}(k)+\nabla_k\,\phi(k) \tag{3.293}$$

The total Berry curvature (2π times the Chern number)

$$\begin{aligned}\iint_{\mathrm{BZ}} d\,k\,\Omega_{-}&=\int\int_{D_I} d\,k\,\nabla\times\mathcal{A}_{-}{}^{(I)}+\int\int_{D_{\mathrm{II}}} d\,k\,\nabla\times\mathcal{A}_{-}{}^{(\mathrm{II})}=\oint_{\partial D_I} d\,k\,\mathcal{A}_{-}{}^{(I)}+\oint_{\partial D_{\mathrm{II}}} d\,k\,\mathcal{A}_{-}{}^{(\mathrm{II})}=\oint_{\partial D_I} d\,k\,\mathcal{A}_{-}{}^{(I)}-\oint_{\partial D_I} d\,\mathrm{k}\mathcal{A}_{-}{}^{(\mathrm{II})}=\\ &\oint_{\partial D_I} d\,k\left(\mathcal{A}_{-}{}^{(I)}-\mathcal{A}_{-}{}^{(\mathrm{II})}\right)=-\oint_{\partial D_I} d\,k\,\nabla_k\,\phi(k)=-\int_0^{2\pi} d\,\theta\,\partial_\theta\,\phi=-[\phi(\theta=2\,\pi)-\phi(\theta=0)]=\phi(\theta=0)-\phi(\theta=2\,\pi)\end{aligned} \tag{3.294}$$

$$\phi(\theta=0)-\phi(\theta=2\,\pi)=2\,\pi\,n \tag{3.295}$$

Therefore, the Chern number is quantized.

For the model we considered here:

$$\mathcal{H}_0(k)=0 \tag{3.296}$$

$$\mathcal{H}_x(k)=\Delta\,\sin(k_x) \tag{3.297}$$

$$\mathcal{H}_y(k)=\Delta\,\sin\left(k_y\right) \tag{3.298}$$

$$\mathcal{H}_z(k)=-2\,t\cos k_x-2\,t\cos k_y-\mu \tag{3.299}$$

If we choose the boundary between D_I and D_{II} to be a very small circle ($k\sim 0$)

$$\mathcal{H}_x(k)=\Delta\,\sin(k_x)\approx\Delta\,k_x+O\left(k^2\right) \tag{3.300}$$

$$\mathcal{H}_y(k)=\Delta\,\sin\left(k_y\right)\approx\Delta\,k_y+O\left(k^2\right) \tag{3.301}$$

$$\mathcal{H}_z(k)=-2\,t\cos k_x-2\,t\cos k_y-\mu=-2\,t-\mu+O\left(k^2\right) \tag{3.302}$$

$$e^{i\,\phi(k)}=\frac{\frac{\mathcal{H}_z+\left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k)+i\,\mathcal{H}_y(k)}}{\left|\frac{\mathcal{H}_z+\left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k)+i\,\mathcal{H}_y(k)}\right|}=\frac{\frac{1}{\mathcal{H}_x(k)+i\,\mathcal{H}_y(k)}}{\left|\frac{1}{\mathcal{H}_x(k)+i\,\mathcal{H}_y(k)}\right|}=\frac{\left|\mathcal{H}_x(k)+i\,\mathcal{H}_y(k)\right|}{\mathcal{H}_x(k)+i\,\mathcal{H}_y(k)}=\frac{\left|\Delta\,k_x+i\,\Delta\,k_y\right|}{\Delta\,k_x+i\,\Delta\,k_y}=\frac{\left|k_x+i\,k_y\right|}{k_x+i\;k_y}=\frac{|k\,||\,e^{i\,\theta}\,|}{|k\,|\;e^{i\,\theta}}=\frac{1}{e^{i\,\theta}}=e^{-i\,\theta} \tag{3.303}$$

$$\phi(k)=-\theta \tag{3.304}$$

$$\iint_{\mathrm{BZ}} d\,k\,\Omega_{-}=\phi(\theta=0)-\phi(\theta=2\,\pi)=0-(-2\,\pi)=2\,\pi \tag{3.305}$$

$$C=\frac{1}{2\,\pi}\iint_{\mathrm{BZ}} d\,k\,\Omega_{-}=1 \tag{3.306}$$

3.13.5. Marginal case: $\mu = 0$

Two Dirac points at k=(0,π) and (π,0). Not an insulator. No topological index.

3.13.6. case III: $0 < \mu < 4\,t$

For $0<\mu<4\,t$, $\mathcal{H}_z>0$ at k=(π,π), and $\mathcal{H}_z<0$ for all three other points.

Use a small circle centered at (π,π) to cut the system into two parts. Inside the circle, near (π,π), we use u^{II} and outside the circle, near (0,0) we use u^I.

Chern number C=1.

3.13.7. Marginal case: $\mu = 4\,t$

Dirac points at k=(π,π). Not an insulator. No topological index.

3.13.8. case IV: $\mu > 4\,t$

All the four special points has $\mathcal{H}_z < 0$. We just use u^I for the whole BZ. No singularity. C=0

3.13.9. case IV: $\mu > 4\,t$

All the four special points has $\mathcal{H}_z < 0$. We just use u^I for the whole BZ. No singularity. C=0

3.13.10. the top band?

The top band has the opposite Chern number $C_+ = -C_-$.

In fact, one can prove that for any tight-binding models, the total Chern number for all the bands is always 0.

So here, we have $C_+ + C_- = 0$.

3.13.11. Summary

- This model has four phases. Two topological phases with C=+1 and two trivial insulator phase with C=0.
- A topological phase and the trivial insulator phase are separated by a phase transition point, which is known as a topological phase transition.
  - Across the topological phase transition, the topological index changes its value
  - Across a topological transition, the insulating gap closes and then reopens (generically true)
  - This is actually a generic statement: A band can only change its Chern number by crossing with another band. i.e. At the topological transition point, the system must be a metal or a semi-metal (with no insulating gap).
- Gap closing is a necessary condition for a topological transition, but it is not a sufficient one. One may close and reopen the gap without changing the topological index. e.g. the μ=0 point here.

3.14. Some properties of the Berry curvature $\mathcal{F}$ (we will limit our discussions to 2D systems)