The Euler characteristic of a square

There is a rule how to partition a square into $\Delta$ pieces

- The rule says the pieces must fit together along the edges
- Bad examples:
  - No overlapping allowed
  - The vertex of a $\Delta$ cannot touch the edge of another $\Delta$

Let's count the following elements:

- Faces $f$: 8
- Edges $e$: 16
- Vertices $v$: 9

Now we calculate $f - e + v = 8 - 16 + 9 = 1$

The partitioning of a figure $K$ into $\Delta$s following the above rule is called a triangulation of $K$.

The number $f - e + v$ is called the Euler characteristic $\chi(K)$:

$$\chi(K) = f - e + v$$

Problem: Calculate Euler characteristic of

Answer: $f - e + v =$
So how you noticed does not matter how you triangulate the answer for $f(x)$ is the same.

But what if we date the a squire into a billion of $\Delta$s? We cannot simply count it.

Example: Theorem $f(\square) = 1$

Consider any $\Delta$ation

If you observe a process of deformation you will find that we always do it by two ways:

$\Delta$eform it

remove 1 $\Delta$

$\Delta$eform it
But in both cases

\[ f - e + v \] is constant!

B/c any Datia of a square is obtained as follows:

\[ f = 2 \]
\[ e = 5 \]
\[ v = 4 \]

\[ f - e + v = 1 \]

We add some triangular as above and deform the resulting into a square: \( \Rightarrow \) any triangulation has \( f - e + v = 1 \). Eop (btw we proved it by induction) starting with \( f = 2 \)

Once we know \( f(\square) = 1 \), we can say that \( \chi(\text{polygon}) = 1 \) on the plane.

Proof:
After we triangulate a polygon we can add a \( \Delta \) and deform the resulting figures to a \( \square \).

\[ \chi(\square) = 1 \]

Next we switch to other surfaces: sphere and torus.
Now we can have a patchwork on the surface of torus or sphere to produce a similar triangulation.

What is $\chi(\text{sphere})$ and $\chi(\text{torus})$?

**Theorem:** $\chi(\text{sphere}) = 2$ and $\chi(\text{torus}) = 0$

I only prove it for a sphere.

Consider a portion of the sphere and let's remove one $\Delta$.

Remove a triangle from the triangulation, then stretch the resulting figure into a flat figure on the plane.

Since the sphere with minus one $\Delta$ can be stretched to the plane. This figure is equal to the large triangle with $\chi(\text{polygon}) = 1$.

Notice the number of $e$ and $\sigma$ remains the same but the number of faces $f$ is changed by 1.

$$\chi(\text{sphere}) = \chi(\text{sphere} - \Delta) + 1 = 2$$

EOP
In topology, we consider two figures to be different if we cannot transform those via elastic deformations.

But what if a figure has holes?

Example of non-closed surfaces:

(a) it has an edge
(b) the surface has singularities

Let's introduce a surface with a hole(s)

A hole is called genus.

Using this notation, we can write the Euler characteristics as:

\[ \chi(S_0) = 2 \quad \chi(S_1) = 0, \quad \text{so what's } \chi(S_g)? \]
I'm going to skip the proof but here is the theorem:

\[ \chi = 2 - 2g \]

for a surface with a boundary \( b \). Let's test this formula:

Fun questions: 1) How many holes or what is genus for this Fig.

2) What is genus of this figure (Klein bottle)?
Q: Is there any connection between $I(z_g)$ and local curvature of a surface?

\[ \frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad y = ax^2 \quad \frac{x^2}{a^2} - \frac{y^2}{b^2} = 1 \]

Those 3 figures a called Conic Sections

The reason we call it Conical b/c those are cross-sections of a cone by a plane

Flow chart of intersections of a double cone and a plane from various positions
How to quantify curvature?

1. **Tangent Plane**

   - **The protocol is simple**
     - Cut the figure by a plane which is going through the point $P$.
   
   - Then do this again for the second time:
     - Draw a tangent line to the obtained cut curves at point $P$.
     - Draw a plane which includes $P$ and 2 tangent lines. This plane is called the tangent plane.
   
   - The way to observe the curvature of the surface $S$ is to shift this plane up and down at $P$, like this:
For the convex surface
the result is the same.

But if our surface
contains a saddle point
The result is very
different.

Now we can say that every point on the oriented
surface of a sphere is elliptical.

But every point on the surface
of a hyperboloid is hyperbolic.

Q: Can the nature of a surface point change?
A: Yes!

Consider a ball made of clay. Every point on the surface of the ball is an
elliptic point. But if we press it with our fingers and make an indentation,
then hyperbolic points appear on the indented region of the surface. In this
process of changing from convexity to concavity, parabolic curving appears
at the moment where convexity changes into concavity. If we move even
slightly away from this moment, parabolic curving immediately changes to
elliptic or hyperbolic curving. Thus, we can say that parabolic curving is
unstable.
Problem: What surface changes its curving in the following way:

\[ \elliptic \rightarrow \parabolic \rightarrow \hyperbolic \]

As you noticed, a point on any surface can be characterized by those 3 categories. But can we measure the curvature quantitatively?

**Enter the GAUSSIAN CURVATURE**

The way we are going to calculate the curvature is to map a point \( P \) on the surface \( S \) to the unit sphere area

\[
K(P) = \lim_{\sigma \to P} \frac{\text{area of } \sigma}{\text{area of } \sigma'}
\]
Gauss - Bonnet theorem

Let's calculate Gaussian curvature of a sphere, since a sphere has a constant radius $R$,

$$K(P) = \frac{1}{r^2}$$

$\Rightarrow$

To arrive at this conclusion we map the sphere to the unit sphere by the transformation with a similarity ratio

$$= \frac{1}{R^2} \left[ \frac{\sqrt{r^2 - 1}}{1 + \sqrt{1 - r^2}} = \frac{1}{R^2} \right]$$

In general

$$K = \frac{1}{R_1} \cdot \frac{1}{R_2}$$

two most extremes

Intuitive picture of a gaussian mapping

$\Rightarrow$

Imagine that the surface is made of rubber. The mapping of a small region $\sigma$ by the $G$-map to the unit sphere is equivalent to cutting out $\sigma$ off the surface $S$.

Next we stretch and shrink it to the curving and then "gluing" it into the unit sphere.
Simply, $S$ is a cut into small pieces and then glued into the unit sphere after stretching, shrinking and reversing of each piece.

**Gauss - Bonnet theorem**

First recall we can deform the closed surface in a concave and convex manner.

Pushing a certain part causes another area to lose its convexity and even become dented inwards.

If the sphere is deformed and some part of it starts having a greater Gaussian curvature, then the curvature of some other parts of the surface will decrease.

Now the theorem itself:

The total sum of the Gaussian curvature $K(\sigma)$ over a surface is equal to the Euler characteristic $\chi$ of the surface $\times 2\pi$.

$$\frac{1}{2\pi} \int K(\sigma) \, d\sigma = \chi(S)$$
We will not prove the theorem, but let us verify it on a sphere \( K(p) = \frac{1}{r^2} \)

\[
\frac{1}{2\pi} \int_S K(p) \, d\sigma = \frac{1}{2\pi} \cdot \frac{1}{r^2} \cdot \int d\sigma = \frac{1}{2\pi} \cdot \frac{1}{r^2} \cdot 4\pi r^2 = 2!
\]

Recall \( X(S_0) = 2 \)

The fundamental result:

\[
\frac{1}{2\pi} \int_S K(p) \sqrt{\sigma} = X(S_g) = 2 - 2g
\]

Vector Fields on Surface

Here is the wind blowing on the sphere

The same on torus

Q: What's the difference?

BTW: \( S(t) = [x(t), y(t)] \) \( \Rightarrow K = \frac{x'(t)y''(t) - y'(t)x''(t)}{(x'(t)^2 + y'(t)^2)^{3/2}} \)
Imagine that the surface is a field with attenuating regions of concavity and convexity and with small vectors in them.

The places where flow stops is called a critical point.

Very generally we can think of what critical points are possible?

Check this figure:

If you spend enough time you can discover that the only critical points are:

Table of possible critical points:
Let's introduce a new tool: the index of a critical point.

E.g., if the top of a mountain is as flat as the top of a table, the fallen rain will collect on those flat areas. In such a case the critical points are everywhere.

Now think of a flow of H2O entering & leaving the critical point.

To calculate the index of the critical point, draw a closed path around it, which contains only one critical point.

Move around the path and measure the direction of the flow at each point.

Since the wind directions revolve once around the circle counter-clockwise we assign the index $P = +1$.
Let us discuss the way you set index again and in a little more detail.

The procedure to follow:

1. Remember to choose a starting point for your walking around say A, then we will walk always counterclockwise:
   \[ A \rightarrow B \rightarrow C \rightarrow D \rightarrow A \]

2. Determine the direction of the vector field at each of the point A ↑, B ↓, C ←, D → etc.

3. Bring those vectors to the special point whose index you try to define.

4. Observe the direction and the number of times you have to move around \( A \rightarrow B \rightarrow C \rightarrow D \rightarrow A \). This number and its sign is your index, \( i(P) \).
What about the critical point index here?

\[ i(P) = -1 \]

**General protocol:** Draw a circle around a critical point \( P \), and go around counter clockwise, observe change in the direction of a vector.

If the direction of the vector revolves \( n \) times we say \( i(P) = +n \).

Otherwise \( i(P) = -n \).

Next page figure shows few interesting examples:
Examples of critical points and their indices.

Here is the very important theorem

**THE POINCARE - HOPF THEOREM**

Let $S_g$ be a closed surface. For any vector field on $S_g$ with finitely many critical points, the sum of the critical point indices $i(p)$ is equal to the Euler characteristic of $S_g$

$$\sum i(p) = 2 - 2g$$
Few comments are due:

*if the surface is a sphere then \( \chi(S_0) = 2 \)

What can we say about the surface?

Apply the P-H theorem we can immediately say that somewhere on the Earth there are 2 and only 2 points where there is no wind.

Consider another example, a dipolar magnetic monopole on the surface of the sphere.

The critical index of this point is \( i(P) = +2 \)

It means there's the only one critical point for this kind of vector field.

Or there can be only ONE dipole magnetic monopole on Earth. Now you can try to search for it.
Here is another example of a "sphere"

This vector field has 4 critical points:
- 2 at peaks A & B  \( i(A) = i(B) = +1 \)
- at pass C  \( i(C) = -1 \)
- point D where water gathers  \( i(D) = +1 \)

The sum of the indices \( \sum i(A, B, C, D) = +1 +1 -1 +1 = +2 \)
\( \chi(S_0) = 2 \) as well.

Now let's consider torus \( S_1 \) with \( \chi(S_1) = 0 \)

This means there is a vector field with no critical points, or all critical point indices can be only compensated, so their sum is zero!
But what if the rainfall vector field drops on the torus

Again we have 4 critical points.

Now we can generalize it to any figure with \( n \) -holes:

\[
\begin{array}{c|c}
\text{critical point} & \text{index} \\
\hline
\text{peak} & 1 \\
\text{saddle} & -1 \\
\text{saddle} & -1 \\
\text{saddle} & -1 \\
\text{valley} & 1 \\
\end{array}
\]

the sum of indices of critical points: \( 2 - 2g \)
SUMMARY

\[ X(\text{Sing}) = 2 - 2g = \frac{\sum i(\omega)}{s_g} = \frac{1}{2\pi} \oint K(P) d\sigma \]

Let me now to tell you something about e-in quantum materials

- \( i = \) singularity in E(\epsilon) dispersion
- \( K(P) = \) curvature = Berry potential
- \( g = 1 = \) because of the periodic boundary conditions

\[ X(S_1) = 0 \]
So far in our discussion we had a missing factor called \( \varphi \)-phase of the \( |\psi\rangle \) function.

\[
|\psi\rangle \rightarrow |	ilde{\psi}\rangle = e^{i\varphi} |\psi\rangle \Rightarrow <\varphi | \tilde{\Omega} | \psi\rangle = <\tilde{\varphi} | \tilde{\Omega} | \tilde{\psi}\rangle
\]

This works \( \hbar / c \) doesn't act on \( \varphi \), which is just a number of magnitude 1.

But there are some observables which are not expectation values of the operator \( \tilde{\Omega} \) and this arbitrary phase plays the role of an observable.

This happens when our hamiltonian \( H \) has a parameter dependence.

In this case \( \varphi \) is called a geometric phase which describes how the wave function depends on the parameters related to geometric features of the system.

\( \varphi \) In a truly isolated system there is no \( \varphi \) Berry phase.
Berry phase and all that

\[ \hat{H}(\varphi) |\Psi_0> = \epsilon |\Psi_0> \]

\( \varphi \) is a some parameter

When solving the Schrödinger equation \( \varphi \) appears in the form \( e^{i\varphi} \) for the ground state solution.

Note: if we deal with analytical solution \( \varphi = 0 \)

if numerical, often use \( \varphi \) as random number.

Suppose we have 2 different ground states for \( \varphi_1 \) with the phase \( \varphi_1 \)

\( \varphi_2 \)

And let's try to explicitly remove the phase \( \varphi \) for each ground state

e.g. \( |\Psi_{g_1}> \rightarrow |\tilde{\Psi}_{g_1}> = e^{-i\varphi_1} |\Psi_{g_1}> \)

\( |\Psi_{g_2}> \rightarrow |\tilde{\Psi}_{g_2}> = e^{-i\varphi_2} |\Psi_{g_2}> \)

this is known as choosing a gauge

The overlap of the two phase-corrected functions

\[ \langle \tilde{\Psi}_{g_1}, \tilde{\Psi}_{g_2} \rangle = e^{i(\varphi_1 - \varphi_2)} \langle \Psi_{g_1}, \Psi_{g_2} \rangle \]
BERRY PHASE and all that

But since we agreed to remove all the phase dependence the left side must be only the magnitude \(|\langle \psi_1 | \psi_2 \rangle|\)

which allows us to define the relative phase \(\Delta \psi_{12}\) as:

\[
\frac{e^{-i \Delta \psi_{12}}}{\langle \psi_1 | \psi_2 \rangle} = \frac{\langle \psi_{q_2} | \psi_{q_1} \rangle}{\langle \psi_{q_1} | \psi_{q_2} \rangle}.
\]

or

\[
\ln e^{-i \Delta \psi_{12}} = \ln (\cdots) \quad \text{or} \quad -i \Delta \psi_{12} = \ln (\cdots)
\]

\[
\Delta \psi_{12} = -\text{Im} \left[ \ln \frac{\langle \psi_{q_1} | \psi_{q_2} \rangle}{\langle \psi_{q_1} | \psi_{q_2} \rangle} \right]
\]

Now let's consider a small difference in \(q_1 \to q_2\)

\[
q_2 = q_1 + \delta q \to 0
\]

\[
e^{-i \Delta \psi_{12}} = \frac{\langle \psi_{q_2} | \psi_{q_1 + \delta q} \rangle}{\langle \psi_{q_1} | \psi_{q_2 + \delta q} \rangle}.
\]

\[
\Delta \psi_{12} = \langle \psi_{q_2} | \psi_{q_1 + \delta q} \rangle \cdot \Delta q + \langle \psi_{q_1} | \psi_{q_2 + \delta q} \rangle
\]

\[
-\Delta \psi_{12} = \langle \psi_{q_2} | \Delta | \psi_{q_1} \rangle \cdot \Delta q \Rightarrow \delta \psi = i \langle \psi_{q_2} | \Delta | \psi_{q_1} \rangle
\]
Berry phase and all that.

And now we can calculate Berry phase:

$$\tilde{\gamma} = \oint d\mathbf{q} = i \oint \langle \tilde{\psi}_q \mid \nabla \tilde{\psi}_q \rangle \cdot d\mathbf{q}$$

If we ever want to measure the B.p. we must assure that it's gauge invariant.

Let's verify this:

$$\Phi_q \rangle = e^{-i \varphi(q)} \langle \psi_q \rangle$$

$$\nabla_q \langle \tilde{\psi}_q \rangle = \left[ -i \nabla_q \varphi(q) \right] e^{-i \varphi(q)} \langle \psi_q \rangle + \langle \tilde{\psi}_q \rangle$$

Now the B.p. is:

$$\tilde{\gamma} = \oint d\mathbf{q} \langle \tilde{\psi}_q \mid \nabla \tilde{\psi}_q \rangle \cdot d\mathbf{q} = \oint \langle \tilde{\psi}_q \mid e^{-i \varphi(q)} \nabla_q \psi_q \rangle \cdot d\mathbf{q} + \oint \int \oint \nabla_q \varphi(q) \cdot d\mathbf{q}.$$
\[ \oint \psi^* \psi \, dq = \psi(A) - \psi(B) = \gamma \]

Returning to the original value of \( \gamma \):

\[ \gamma = i \oint_c \langle \psi_\varphi | e^{-i \varphi(y)} \nabla | \psi_\varphi \rangle \]

\[ = i \oint_c \langle \psi_\varphi | e^{-i \varphi(y)} e^{i \varphi(y)} \nabla | \psi_\varphi \rangle \, dq = \]

\[ = i \oint_c \langle \psi_\varphi | \nabla | \psi_\varphi \rangle \, dq = \gamma \]

\[ \text{Eop} \]

\( \gamma \) or B. ph. is locally phase invariant and as such is observable.
Berry phase and all that

Another look at gauge invariance

If the system is easily represented by a discrete set of ground states we can try the original definition:

\[ \Delta \psi_{12} = -\text{Im} \left[ \ln \left( \langle \psi_{g_1} | \psi_{g_2} \rangle \right) \right] \]

Here \( q_0 = g_{N+1} \)

and \( q_{i+1} = q_i + dq \)

Then we can write down

\[ \Delta \psi = -\text{Im} \left[ \sum_{i=0}^{N} \ln \left( \langle \psi_i | \psi_{i+1} \rangle \right) \right] = \sum \lambda_n = \ln \prod \]

\[ = -\text{Im} \left[ \ln \left( \prod_{i=0}^{N} \langle \psi_i | \psi_{i+1} \rangle \right) \right] \]
But is the discrete B.P. locally gauge invariant?

To glean we introduce

\[ |\tilde{\Psi}_q\rangle = e^{-i\gamma(q)} |\Psi_q\rangle \]

Consider \( \prod |\tilde{\Psi}_q| |\tilde{\Psi}_{q+1}\rangle \equiv |\Psi_{19}, q_{19}, \ldots, q_{19}, q_{19+1}\rangle e^{i\gamma(q)}, e^{-i\gamma(q)} \equiv 1 \)

so the phases cancel out between the successive steps b/c they arise from bra and ket with the same index and for \( q_{19} \) and \( q_{19+1} \) phase is also the same, as they represent the same end point.

I want to stress only \( \Pi \) or \( \oint \) is locally gauge invariant, the integrand itself NOT!

- The value of \( \gamma \) depends on the contour of integration.

Now I want to consider a very special case: when the parameter \( q \) is REAL.
If this is the case we can introduce two quantities:

\[ \mathbf{A}(\hat{q}) = i \langle \psi_\gamma | \mathbf{\hat{D}}_\gamma \psi_\gamma \rangle \rightarrow a 3 \text{-component vector} \]

\[ \Omega_{\alpha\beta}(\hat{q}) = \frac{\partial A_\beta(\hat{q})}{\partial \hat{q}_\alpha} - \frac{\partial A_\alpha(\hat{q})}{\partial \hat{q}_\beta} \]

And

\[ = i \left[ \frac{\partial}{\partial \gamma_\alpha} \left( \frac{\partial}{\partial \gamma_\beta} \langle \psi_\alpha | \psi_\beta \rangle \right) - \frac{\partial}{\partial \gamma_\beta} \left( \frac{\partial}{\partial \gamma_\alpha} \langle \psi_\alpha | \psi_\beta \rangle \right) \right] = \]

\[ \text{B/c } \gamma \text{ is real} \]

\[ = -2 \text{ Im } \langle \frac{\partial \psi_\alpha}{\partial \gamma_\alpha} | \frac{\partial \psi_\beta}{\partial \gamma_\beta} \rangle \]

We can also associate the elements of the tensor with 3 \text{ comp vector } \Omega_{\alpha\beta}

by the cyclic permutation of indices, e.g., \[ \Omega_{xy} \rightarrow 3 \text{ component of } \Omega_{\gamma} \]

or \[ \Omega_{\alpha\beta} = \epsilon_{\alpha\beta\gamma} \Omega_{\gamma} \rightarrow \text{ the Levi-Civita tensor} \]
Berry Phase and all that

Thus now I can write down \( \mathbf{\Omega} \) as the curl of \( A \)

\[
\mathbf{\Omega} (\vec{q}) = \frac{\partial A_\beta (\vec{q})}{\partial q^\alpha} - \frac{\partial A_\alpha (\vec{q})}{\partial q^\beta}
\]

\[
\mathbf{\Omega} (\vec{q}) = \nabla_\vec{q} \times A (\vec{q})
\]

And finally:

Berry connection or Berry potential

\[
\gamma = \oint\nabla_\vec{q} \times A (\vec{q}) \cdot d\vec{q} = \oint s \left[ \oint \nabla_\vec{q} \times A (\vec{q}) \cdot ds \right]
\]

Berry curvature

\[
\gamma = \oint s \mathbf{\Omega} (\vec{q}) \cdot d\vec{s}
\]

Here \( S \) is the surface enclosed by \( S \) and \( d\vec{s} \). The surface unit vector points in the right hand rule direction.

To connect you to the perturbation theory, I can show how to calculate \( \gamma \) from the perturbation theory, i.e., if \( |q^\alpha \rangle \in E_i^{(0)} \) is ground state and
BERRY PHASE and all that

\( \Psi_n^{(n)} \) and \( \epsilon_n^{(n)} \) is the excited state

we have \( \left| \frac{\partial \psi^{(0)}}{\partial \mathbf{\alpha}} \right| = \sum_{n=0}^{\infty} \left| \psi_n^{(n)} \right| \).

\( \langle \psi_n^{(n)} | \frac{\partial^2 \mathcal{H}}{\partial \mathbf{\alpha} \partial \mathbf{\beta}} | \psi_{n_0}^{(n_0)} \rangle \)

\( \epsilon_n^{(0)} - \epsilon_n^{(n)} \)

from this the Berry curvature \( \Omega_{\alpha \beta}(\mathbf{q}) \)

\( = -2 \text{Im} \left\{ \sum_{n=0}^{\infty} \left| \psi_n^{(n)} \right|^2 \mathcal{H}_{\alpha \beta} \left| \psi_n^{(n)} \right| \right\} \)

\( \langle \psi_{n_0}^{(n_0)} | \frac{\partial \mathcal{H}}{\partial \mathbf{\alpha}} | \psi_{n_0}^{(n_0)} \rangle \)

\( \left( \epsilon_n^{(0)} - \epsilon_n^{(n)} \right) \)

The advantage, we don’t need to calculate derivatives of \( \Psi_n^{(n)} \) but only \( \Psi_n^{(n)} \). But you need to sum up over all \( \left| \Psi_n^{(n)} \right| \)

For fun let’s calculate B. ph. of a molecule, or a triangular lattice solid.
EXAMPLE

Thus we have several configurations:

\[ \begin{array}{cccc}
  a & b & c & d \\
\end{array} \]

\[ a = d \]

Recall \( \gamma = - \text{Im} \ln \prod_0^N <\psi_i | \psi_{i+1}> \) in the 3-atomic molecule the states are:

\[ \begin{align*}
  |\psi_a> &= |\psi_d> = \frac{1}{\sqrt{2}} |1\rangle \\
  |\psi_b> &= \frac{1}{\sqrt{2}} (e^{2\pi i/3}) \\
  |\psi_c> &= \frac{1}{\sqrt{2}} (e^{\pi i/3\pi i}) \\
\end{align*} \]

\[ \gamma = - \text{Im} \ln \left[ <\psi_a | \psi_b> <\psi_a | \psi_c> <\psi_c | \psi_d> \right] = - \frac{\pi}{2} \]

So \( \gamma = -\frac{\pi}{2} \).

And the Chern index is \( c = \left| \frac{\gamma}{2\pi} \right| = \frac{1}{2} \).

More on Chern number follows later.
Example 2

Aharonov–Bohm effect as a Berry phase

Our quantum system is made of an electron and the potential \( V(r) \) which localizes it.

\[
H \psi(r) = \left[ -\frac{\hbar^2}{2m_e} \nabla^2 + V(r) \right] \psi(r) = E \psi(r)
\]

Imagine we shift the origin of the confining potential by \( \bar{R} \) so the Hamiltonian is \( \bar{R} \)-parameter dependent.

\[
\hat{H}_{\bar{R}} \psi_{\bar{R}}(r) = \left[ -\frac{\hbar^2}{2m_e} \nabla^2 + V(r-\bar{R}) \right] \psi_{\bar{R}}(r) = E_{\bar{R}} \psi_{\bar{R}}(r)
\]

Translational invariance requires:

\[
\psi_{\bar{R}}(r) = \psi(r-\bar{R}) \quad E_{\bar{R}} = E
\]

Now I will transport the electron \( \psi_{\bar{R}} \) around a closed path \( C \) which is far far away from the region with magnetic field.
The new Hamiltonian is now

\[ \hat{H}_R = \frac{1}{2m_e} \left[ -i \hbar \nabla_r + \frac{e}{c} A(r) \right]^2 + V(r-R) \]

The new w.f. for this Hamiltonian

\[ \psi_R(r) = e^{\frac{i e}{\hbar c} \int_R^r A(r') \, dr'} \psi(r-R) \]

with the phase

\[ \psi_R(r) = -\frac{e}{\hbar c} \int_R^r A(r') \, dr' \]

which depends on \( \text{path} \) and is not well defined.

Let's try to restore the simple value of it by selecting a good path for integration.

In other words, since \( A(r) \) is 0 for the region where \( B \neq 0 \) thus we want to stay away from the \( B \)-field area.

Let us calculate Berry connection:

\[ A(r) = i \left< \psi_R \right| \nabla_r \psi_R > = \frac{e}{\hbar c} A(r) + i \int \psi^* (r-R) \nabla_r \psi(r-R) \, dr \]

\[ \rightarrow \quad \text{it is} \quad 0 \quad \text{to prove} \]
First I define \( r' = r - R \) and use the chain rule to switch the variables:

\[
\int \psi^*(r') \nabla_{r'} \psi(r') \cdot dr' \left( \frac{2r'}{\hbar^2} \right) = -\int \frac{\psi^*(r')}{\sqrt{2}} \nabla_{r'} \psi(r') dr'
\]

\[
\sim \text{ expectation value of momentum in } \psi(r')
\]

which is for a bound state \( \Phi = 0 \)

What remains is to calculate the B.P.

\[
\gamma = -\frac{e}{\hbar c} \oint A(R) dR = -\frac{e}{\hbar c} \iint_S (\nabla \times A(R)) \cdot dS
\]

\[
= -\frac{e}{\hbar c} \oint_S \mathbf{B} \cdot d\mathbf{S} = -2\pi \frac{\Phi}{\Phi_0} = \frac{2.067933 \times 10^{-15} \text{ Wb}}{\Phi_0} = \hbar c/e \equiv \text{ QUANTUM}
\]

In other words, \( \gamma \sim \Phi \) of the \( \mathbf{B} \).

B.P. is sampling the single "dot" region of \( \mathbf{B} \) and is sensed by \( 1\psi \) transported around this point. This phase was measured in the change of the interference pattern in the double slit experiment.
Topological Meaning

① Note, A-B effect is topological.
This happens b/c the wave function is defined in the plane minus the origin, i.e., a sheet with a hole in it. The result is the same if we place an infinite thin flux tube of \( \mathcal{D} \) at \( r=0 \). We punctured a hole in the manifold!

Recall electromagnetism has U(1) symmetry, which has the same topology as the circle \( S^1 \).
Mathematically, we map \( S^1 \) to a path around a hole, \( \pi_1(S) = \mathbb{Z} \).
This mapping is characterized by an integer winding number.

Geometrical phases only exist when the space is NOT simply connected.

② Note if the ground state \( |\Psi_0 \rangle \) is \( N \)-degenerate, we need to use non-Abelian Berry connection.
SUMMARY OF A-B.

D Recall in magnetostatics:
\[ \oint \vec{B} \cdot d\vec{s} = \oint (\nabla \times \vec{B}) \cdot \hat{n} \, dS \]

D and also we can write
\[ \vec{B} = \nabla \times \vec{A} \]

\[ B_x = B_y = 0 \quad A_x \neq 0 \quad A_y \neq 0 \]

\[ \oint \vec{A} \cdot d\vec{s} = B \cdot \pi r^2 = \text{FLUX} \]

D Berry etc.
\[ \oint \langle \nabla \lambda \nabla \lambda^* \rangle \, d\lambda = \oint A(\lambda) \cdot d\lambda \equiv \oint \vec{A} \cdot d\vec{s} \]

\[ \equiv A(\lambda) \equiv \text{Berry potential} \]

Berry phase \( \varphi = - \text{Im}(\text{total Berry curvature}) \)
also \( \oint A(\lambda) \, d\lambda = \text{FLUX OF BERRY CURVATURE} \)

\[ \Rightarrow \text{Berry phase} = - \text{Im} \left\{ \text{FLUX OF BERRY CURVATURE} \right\} \]

\[ = \text{SUM OF CRITICAL INDEXES OF TOPOLOGICAL CHARGES OF} \]
What is a Chern number?

Quantum Hall Effect Explained

1. Let us very briefly introduce Berry phase for electrons in a crystal.

Inside a periodic lattice an electron is described by a periodic (Bloch) wave function

\[ \Psi_k(r) = e^{i k \cdot r} \]
\[ \Psi_k(r) = e^{i (\vec{k} + \vec{n}a) \cdot \vec{r}} \]

\[ U_k^{(n)}(\vec{r}) = U_k^{(n)}(\vec{r} + \vec{n}a) \]

\( n \) - is a band index

The Hamiltonian is

\[ \mathcal{H}_k(p, r) = \frac{1}{2m_e} \left( -i \hbar \nabla_r + h \vec{k} \right)^2 + V(r) \]

and later we will add an electric field as perturbation.

Recap

\[ A_{\alpha}^{(n)}(k) = i \left< U_k^{(n)} \right| \nabla_k U_k^{(n)} \right> \Rightarrow \]

\[ \Omega_{\alpha \beta}^{(n)}(k) = i \left< \frac{\partial U_k^{(n)}}{\partial k_{\alpha}} \right| \frac{\partial U_k^{(n)}}{\partial k_{\beta}} \right> - \left< \frac{\partial U_k^{(n)}}{\partial k_{\beta}} \right| \frac{\partial U_k^{(n)}}{\partial k_{\alpha}} \right> \]

\[ A_{\alpha}^{(n)}(k) = i \left< \nabla_k U_k^{(n)} \right| \nabla_k U_k^{(n)} \right> \]

and \( \gamma^{(n)} = i \oint_C \left< U_k^{(n)} \right| \nabla_k U_k^{(n)} \right> \cdot d\vec{k} \)

C is a closed path in the momentum space or the Brillouin zone of the crystal.

and the path is realized by moving a point \( k \) to the \( k + \delta = \frac{2\pi}{a} \)
Thus \( \mathbf{k} \to \mathbf{k} + \mathbf{G} \) transport loops the electron within the same B.Z.

Now let's place the electron into the field

**QUANTUM**

**HALL EFFECT**

**Experimental**

\[
\frac{R_{xy}}{R_x} = \frac{\delta}{B} \quad R_x = \frac{\delta}{B} \\
\]

Integral Quantum Hall effect = IQHE

Fractional quantum Hall effect = FQHE
Topological properties of IQHE

Geometrical properties of an object in the mathematical space.

E.g. k-space for the electron in the Hilbert space.

The goal is to classify objects based on geometrical properties:
- bending, stretching, and
- forming holes and genuine is NOT!

E.g., how many times the loop winds up before it encloses the point P.

"Answer: 2 times."

Let's try this mathematically:
1st we define the function

$z(t), \ t \in [0, T], \ t \in \mathbb{R}$

$z \in \mathbb{C}$, as usual

$z(t) = |z(t)| \cdot e^{i \varphi(t)}$

Now we can define the integral:

$$Q_I(z) = \frac{1}{2\pi i} \int_0^t \frac{d \bar{z}(t)/dt}{z(t)} \, dt$$

Let's confirm that $Q_I$ is the quantity we want:

$$Q_I(z) = \frac{1}{2\pi i} \int_0^t \frac{d \bar{z}(t)/dt}{z(t)} \, dt =$$

$$= \frac{1}{2\pi i} \left[ \ln(z(t)) \right]_0^t = \frac{1}{2\pi i} \left[ \ln \left( \frac{z(t) e^{i \varphi(t)}}{z(0) e^{i \varphi(0)}} \right) \right] =$$

$$= \frac{1}{2\pi i} \cdot \left( \ln(e^{i \varphi(t)}) - \ln(e^{i \varphi(0)}) \right) =$$

$$= \left[ \varphi(t) - \varphi(0) \right] / 2\pi$$

if $\varphi(t)$ is continuous, i.e. no jump from $2\pi \to 0$ after the turn $\Rightarrow Q_I(z)$ gives the number of turns $\Gamma$!
Most important we classify all possible paths in 2D:

Obviously \( Q_1(x) \in \mathbb{Z} \Rightarrow \) is called \( Q_1(x) \) is a \( \mathbb{Z} \)-type topological invariant.

Let's apply this concept to IQHE

For this purpose we rederive Hall conductivity tensor quantum-mechanically in Kubo approximation.

1) Bloch state in a solid is \( \psi_{nk}(x) = \phi_{nk}\) \( e^{ikx} \)
   - \( n \) - band index
   - \( k \) - wave vector

2) Apply 1st order perturbation theory in the weak electric field \( \vec{E} = E_x \cdot \hat{\vec{e}}_x \)
   - the electric potential \( \phi_e(x) = E_x \cdot x = -i \frac{d}{dk_z} \cdot x \)

The perturbed w.f.
\[
|n\rangle = |n_0\rangle - \sum_{m \neq n_0} \langle m_0 | c_0 \frac{d}{dk_z} | m_0 \rangle
\]

\( E_{n_0} \) and \( E_{m_0} \) solutions of unperturbed Hamiltonian.

Let's determine the velocity in \( \vec{y} \)-direction
\[ y = \frac{\langle h | \hat{V} | y \rangle}{\langle h | y \rangle} = \frac{\langle h | \hat{V} y | h \rangle}{\langle h | y | h \rangle} = \frac{\langle h | \hat{V} y | h \rangle}{\langle h | y | h \rangle} - ic \sum_{m \neq h} \langle \text{hol} | V y | \text{mo} \rangle \langle \text{hol} | \frac{d}{dt} | \text{mo} \rangle \langle \text{mo} | h \rangle + h.c.
\]

\[ p_{xy} = \frac{1}{\gamma_{xy}} ?\]

\[ \text{integer?} \]

\[ \sigma_y = \frac{dy}{dt} = -\frac{i}{\hbar} [\hat{H}, y] \left\langle \text{verify from } \frac{\partial y}{\partial t} = \hat{H} y \right\rangle \]

\[ \langle \text{hol} | V y | \text{mo} \rangle = -\frac{i}{\hbar} \left( \langle \text{hol} | H y | \text{mo} \rangle - \langle \text{hol} | y H | \text{mo} \rangle \right) \]

\[ = -\frac{i}{\hbar} \langle \text{hol} | y \rangle \cdot (E_{\text{mo}} - E_{\text{no}}) \]

\[ \uparrow \]

\[ y = -i \frac{2}{\partial y} \]

\[ \langle \text{hol} | V y | \text{mo} \rangle = -\frac{i}{\hbar} \langle \text{hol} | \frac{2}{\partial y} | \text{mo} \rangle (E_{\text{mo}} - E_{\text{no}}) = -\frac{i}{\hbar} \langle \frac{d\text{no}}{d y} | \text{mo} \rangle \cdot (E_{\text{no}} - E_{\text{no}}) \]

for all \( m \neq h \). Insert \( \bullet \) into \( \sigma_y \)

\[ \sigma_y = \langle \text{hol} | V y | \text{no} \rangle + ic \frac{\partial}{\partial x} \sum_{m \neq \text{no}} \langle \text{no} | \frac{d\text{no}}{d y} | \text{mo} \rangle.
\]

\[ \langle \text{mo} | \frac{2}{\partial y} \rangle + h.c. \]

from \( \bullet \)

\[ \langle \text{hol} | V y | \text{no} \rangle = -\frac{i}{\hbar} \langle \text{hol} | \frac{2}{\partial y} | \text{no} \rangle (E_{\text{no}} - E_{\text{no}}) = 0! \]
So finally,
\[ \sigma_y = \frac{i e E_y}{\hbar} \left( \langle \frac{\partial \psi_0}{\partial k_y} \mid \frac{\partial \psi_0}{\partial k_x} \rangle - \langle \frac{\partial \psi_0}{\partial k_x} \mid \frac{\partial \psi_0}{\partial k_y} \rangle \right) \]
and since the plane wave part in \( |\psi_0\rangle = U_{nk}(\vec{x}) e^{i \vec{k} \cdot \vec{x}} \) doesn't contribute, we finally get:
\[ \sigma_y = \frac{i e E_y}{\hbar} \left( \langle \frac{\partial U_{nk}(\vec{x})}{\partial k_y} \mid \frac{\partial U_{nk}(\vec{x})}{\partial k_x} \rangle - \langle \frac{\partial U_{nk}(\vec{x})}{\partial k_x} \mid \frac{\partial U_{nk}(\vec{x})}{\partial k_y} \rangle \right) \]

Linear response theory based on Kubo formalism.

To get current \( I_y \) in the electric field \( E_x \), we add up all the contributions from all occupied states \( U_{nk}(\vec{x}) \).
The transverse current $\neq 0$ if $\frac{\partial U}{\partial k_x}$ and $\frac{\partial U}{\partial k_y}$ are different! and contribution from different $k$, should not cancel.

Now we need to prove that the same Bloch w.f. works for a magnetic field.

Recall the translation operator ($\sigma=0$)

$$T(R_n) = e^{i \vec{R}_n \cdot \vec{D}}$$

$$T(R_n) \cdot f(\vec{x}) = f(\vec{x} + \vec{R}_n) \Rightarrow T(V(\vec{x})) = V(\vec{x} + \vec{R}_n)$$

it also commutes with $\nabla^2$, $h=\frac{1}{2}$, $\ldots$ = $V(\vec{x})$

$$\Rightarrow$$ it commutes with

$$H = -\frac{\hbar^2}{2m} \nabla^2 + eV(\vec{x})$$

$$\Rightarrow$$ eigenstates of $H$ and $T$ are common $\Rightarrow$ exactly Bloch functions

Now we apply an external mag. field $B$
\[ \hat{H}_B = \frac{1}{2m} (i \hbar \nabla + e \hat{A}(x))^2 + e \hat{V}(x) \]

where \( \hat{A}(x) = -\frac{1}{i} \hat{\text{curl}}(\hat{x} \times \hat{B}) \)

up in symmetric gauge

Since \( A(x) \neq A(x + R_n) \), \( T(R_n) \) doesn't commute with \( \hat{H}_B \), but

new \( T_B(R_n) = e^{R_n \cdot (\nabla - \frac{e}{i \hbar} \hat{A}(x))} \)

will commute with \( i \hbar \nabla + e A(x) \). Show this!

But now the problem is:

\[ T_B(R_n) V(x) = e^{R_n \cdot \frac{e}{i \hbar} \hat{\text{curl}}(\hat{x} \times \hat{B})} V(x + R_n) \]

extra phase

Imagine we now move in the loop by applying the operator \( T_B(R_n) \) many times.

\[ \text{area} \tilde{A} = i \frac{e B}{\hbar} \tilde{A} = i 2\pi n \tilde{A} \]

= if integer

\[ \oint A(x) dx = \int \int \delta x A(\tilde{x}) d\tilde{A} = \int \int \delta B d\tilde{A} = 181 \cdot \tilde{A} \cdot \text{sgn}(\tilde{B} \tilde{A}) \]
Finally we calculate the current:

\[ J_y = -e \oint (2\pi)^2 \mathbf{v} \cdot \mathbf{E} \, d\mathbf{k} = \frac{1}{\text{Mag. Bz}} \]

\[ = -e \oint (2\pi)^2 \left( \frac{i \varepsilon E_y}{\hbar} \left( \left\langle \frac{\partial u_{n,k}(\mathbf{x})}{\partial k_y} \right| \frac{\partial u_{n,k}(\mathbf{x})}{\partial k_y} \right\rangle \right) d^2 k = \]

\[ J_y = \frac{e^2}{h} \oint \frac{1}{2\pi i} \left( \left\langle \mathbf{E} \cdot \mathbf{E} \right\rangle - \left\langle \mathbf{E} \cdot \mathbf{E} \right\rangle \right) d^2 k \]

But according to the experimental result, the integral must be integer at the plateaux of the transverse or

\[ \sigma_{xy} = e^2 \hbar / 2m \]
This integer \( n_{\text{Ch}} \) is called the Chern number.

To show that the Chern number is integer we use the Stokes theorem:

\[
\langle 1 | > < 1 | \rangle = \left[ \nabla_k \times \langle \mathbf{U}_n \mathbf{e}(\mathbf{x}) | \mathbf{D}_k | \mathbf{U}_n \mathbf{e}(\mathbf{x}) \rangle \right]_2 = [\nabla_k \times \mathbf{A}_{\text{Berry, } n}(\mathbf{x})]_2
\]

where \( \nabla_k = \frac{\partial}{\partial k} \), and 2 is the 3rd component.

Recall the vector:

\[ \mathbf{A}_{\text{Berry, } n}(\mathbf{x}) \equiv \langle \mathbf{U}_n \mathbf{e}(\mathbf{x}) | \mathbf{D}_k | \mathbf{U}_n \mathbf{e}(\mathbf{x}) \rangle \]

is the Berry connection.

By the Stokes theorem if the integrand is continuous

\[
\delta_{xy} = \frac{\mathbf{J}_x}{E_x} = \frac{e}{\hbar} \cdot \frac{1}{2\pi i} \oint \mathbf{A}_{\text{Berry, } n}(\mathbf{x}) \cdot d\mathbf{x}
\]

\[ \approx \frac{e^2}{\hbar} \cdot \frac{1}{2\pi i} \cdot \Phi_{\text{Berry, } n} \]

Left: Berry Phase
Reminder: Let's go back where we started: our quest for topology in QM.

\[ Q_I(\varphi) = \frac{1}{2\pi i} \int_0^t \frac{dz(t)/dt}{z(t)} \, dt \]

Let's confirm this \( Q_I \) is the quantity we want:

\[ Q_I(\varphi) = \frac{1}{2\pi i} \int_0^t \frac{d}{dt} \left( \ln(z(t)) \right) \, dt = \]

\[ = \frac{1}{2\pi i} \left. \ln(z(t)) \right|_0^t = \frac{1}{2\pi i} \ln \left| \frac{z(t)e^{i\varphi(t)}}{z(0)e^{i\varphi(0)}} \right| \]

\[ = \frac{1}{2\pi i} \left( \ln(\frac{e^{i\varphi(t)}}{\frac{e^{i\varphi(t)}}{e^{i\varphi(0)}}}) \right) = \]

\[ = \frac{1}{2\pi i} \left( \ln(e^{i\varphi(t) - i\varphi(0)}) \right) = \frac{\varphi(t) - \varphi(0)}{2\pi} \]

If \( \varphi(t) \) is continuous, i.e., no jump from \( 2\pi \to 0 \) after the turn \( \Rightarrow Q_I(\varphi) \) gives the number of turns! 

\[ \rightarrow \text{notice if the phase difference} \]
\[ \varphi(t) - \varphi(0) = 2\pi n \text{ integer} \]

\[ \Rightarrow Q_I \text{ is integer!} \]

Let's compare this to \( \sigma_{xy} \):

\[ \sigma_{xy} = \frac{j_y}{E_x} = \frac{e^2}{\hbar} \cdot \frac{1}{2\pi i} \oint A_{\text{Berry}, n}(k) \, dk \]

\[ = \frac{e^2}{\hbar} \cdot \frac{1}{2\pi i} \cdot \varphi_{\text{Berry}, n} = \frac{e^2}{\hbar} \frac{1}{2\pi i} \cdot \varphi(\vec{k}) \]

\[ E_\text{Fermi} = - \frac{1}{k_F} = c_1 = Q_I(\varphi) \]

\[ \text{Fermi surface radius } c_1 \text{ is solid} \text{ in } k \text{-space} \]

\[ \text{a number of turns around a singularity in } E^2/H \text{ units of } e^2/\hbar \]
Crystal electrons in Uniform electric field
from the previous section we described the velocity of a Bloch electron along $y$ as

$$\langle \mathbf{V_y} \rangle = \frac{1}{\hbar} \mathbf{\nabla}_k \mathbf{E}_n(k) - \frac{e}{\hbar} \mathbf{E}_x \mathbf{R}_{xy}^{(n)} \mathbf{E}_y$$

and demonstrated that

$$\sigma_{xy} = \frac{e^2}{\hbar} \mathbf{C}_1^{(n)}$$

where

$$\mathbf{C}_1^{(n)} = \frac{1}{2\pi} \int_{M\mathbf{B}^2} \mathbf{R}_{xy}^{(n)}(k) d\mathbf{k} \, d\mathbf{k}$$

The 1st Chern number

The conclusion is if the 1st Chern number is an integer, the Berry's phase for the path that goes around the magnetic $B^2$ is an integer $\times 2\pi$, which makes the invariant
Why do we need to know about the Chern number?

A: The reason is that now you have a precise way of classifying a property of the surface described by the B. curvature.

Higher Chern numbers can be also defined. But for now the 1st Chern number describes the torus of 2D space that the symmetric nature of the MBZ, arising from periodic boundary conditions.

Here is another argument why the 1st Chern number is integer.

Let's stay in 2D.

\[ \begin{pmatrix} 1 \bar{k}_y \\ \bar{k}_x \end{pmatrix} \]

\[ \bar{k}_x \text{ and } \bar{k}_y \text{ are units of } \pi/a \]
We can perform the Chern number calculation as a line integral along the boundary of the BZ.

\[
\begin{align*}
\text{AB} & \rightarrow \text{BC} \rightarrow \text{CD} \rightarrow \text{DA} \\
\begin{cases}
1 \text{ is } k_x = k_y = \frac{\pi}{a} \\
1 \text{ is } k_x = k_y = -\frac{\pi}{a}
\end{cases}
\end{align*}
\]

\[
2\pi C_1 = \oint \overline{A}^{(n)}(k_x, k_y) \, dk = \]

\[
= \int_{AB} A_x^{(n)}(k_x, \bar{1}) \, dk_x + \int_{BC} A_y^{(1)}(1, k_y) \, dk_y 
+ \int_{CD} A_x^{(n)}(k_x, 1) \, dk_x + \int_{DA} A_y^{(\bar{1}, k_y)} \, dk_y 
= \int_{1}^{1} \left[ A_x(k_x, \bar{1}) - A_x(k_x, 1) \right] \, dk_x 
+ \int_{1}^{1} \left[ A_y(1, k_y) - A_y(\bar{1}, k_y) \right] \, dk_y
\]

if you recall \( A_j^{(n)}(k_x, k_y) = i \langle \psi^{(n)}_k \rangle \)

\[
\frac{\partial}{\partial k_j} \psi^{(n)}_k \quad \text{where } j = x, y
\]
Also recall the states at the opposite sides of the BZ are the same states so they are related by a phase factor

\[ |U_{k_x,1}^{(n)}\rangle = e^{i\Phi_x(k_x)}|U_{k_x,1}^{(n)}\rangle \]

\[ |U_{k_y}^{(n)}\rangle = e^{-i\Phi_y(k_y)}|U_{k_y}^{(n)}\rangle \]

Substituting these expressions into the integral we get

\[ 2\pi C_i^{(n)} = \Psi_x(1) - \Psi_x(\bar{1}) - \Psi_y(1) + \Psi_y(\bar{1}) \]

we can connect the states at the corners of the path:

\[ |U_{k_A}^{(n)}\rangle \rightarrow |U_{k_B}^{(n)}\rangle \rightarrow |U_{k_c}^{(n)}\rangle \rightarrow |U_{k_D}^{(n)}\rangle \]

\[ \rightarrow |U_{k_A}^{(n)}\rangle \]

by employing the phase difference between these states

\[ |U_{\bar{1}}^{(n)}\rangle = e^{i\Phi_y(\bar{1})} |U_{\bar{1}}^{(n)}\rangle = e^{i[\Phi_y(\bar{1}) + \Phi_x(1)]} |U_{\bar{1}}^{(n)}\rangle = e^{i[\Phi_y(\bar{1}) + \Phi_x(1) - \Phi_x(1) - \Phi_y(1)]} |U_{\bar{1}}^{(n)}\rangle = \]

\[ e^{i\Phi_y(\bar{1})} |U_{\bar{1}}^{(n)}\rangle \]
\[ \psi_0 (\bar{1}) + \psi_x (1) - \psi_y (1) - \psi_x (\bar{1}) \]

and by this we end up with the same wave function which is single valued. We must have

\[ e^{i [ \psi_y (\bar{1}) + \psi_x (1) - \psi_y (1) - \psi_x (\bar{1}) ]} \]

\[ = 1 \Rightarrow \psi_y (\bar{1}) + \psi_x (1) - \psi_y (1) - \psi_x (\bar{1}) \]

\[ = 2\pi \ell \quad \ell = \text{integer} \]

This proves that \( \ell \) must be integer.

**Left:** The band structure of a single layer of MoS\(_2\). The highest valence band is shown enclosed in a red rectangle near the Fermi level (zero value on the energy axis). **Right:** The calculated Berry curvature (\( \text{Å}^{-2} \)) for the highest valence band; the white hexagon shows the first Brillouin zone [from S. Fang and E. Kaxiras, *Phys. Rev. B* **93**, 235153 (2016)].
Weyl and Dirac semimetal

The presence of a gap is critical for adiabatic evolution. Can we have a topological phase without a global gap in bulk?

Accidental degeneracy and Dimensions

In electronic band theory of quantum materials: degeneracy at \( \vec{k} \) is governed by symmetry. The dimension of a irreducible repres. at given \( \vec{k} \) is equal to generacy at that point.

But in topo metals band degeneracy arises from topology and closes a gap at \( \vec{k} \) not b/c. of symmetry
The condition for that was investigated by Herring in 1937.

Q: Starting with two bands can we bring these bands into degeneracy by tuning Hamiltonian parameters? e.g., for a system represented by

\[ H(\kappa) = h_0(\kappa) \sigma_0 + h(x) \cdot \vec{b} \]

the details of coupling described by

\[ h(\kappa) = (h_1(\kappa), h_2(\kappa), h_3(\kappa)) \]

of a periodic function of \( \kappa \).

All the info about the topology of the W.S. is encoded in \( 4 - 2\pi^2 \) and periodic functions (\( h_0(\kappa), h_1(\kappa), h_2(\kappa) \), all defined on the whole BZ torus \( \mathbb{T}^2 \)). The function \( h_0(\kappa) \) simply shifts the eigenvalues without affecting the eigenstates \( \Rightarrow \) no effect on topo properties, but it enters the dispersion...
The eigenstates are (2x2 Hamiltonian)

\[ \varepsilon_{\pm}(k) = \hbar_0(c \bar{u}) \pm \sqrt{\hbar_1^2(k) + \hbar_2^2(k)} + \hbar_3^2(k) \]

For a general k point and in the absence of I and TR symmetry

\[ h_j(k) \neq 0 \quad \text{for each } j \], but

\[ \varepsilon_+(k) = \varepsilon_-(k) \quad \text{only if } h_j(c \bar{u}) \quad \text{for each } j > 0 \quad \text{at some } \bar{k} = \bar{k}_0 \]

In 3D I can vary each of the 3 components of \( \bar{k} \) and look for simultaneous zeroes of each \( h_j(c \bar{u}) \), \( j > 0 \).

Here is the construction:

- each of the 3 equations \( h_j(c \bar{u}) = 0 \) describes a 2-D surface in \( k \)-space
- 2 such surfaces intersect along lines
- and those lines may intersect the 3rd surface.
at points without fine tuning.

In general those points appear in pairs and the dispersion can be linearized.

The effective Hamiltonian then at $k_0 + \delta \vec{k}$ is then

$$H(\delta \vec{k}) = E_{k_0} + \hbar \nabla_k h_0(\vec{k}) \cdot \vec{\delta}_0 +$$

$$+ \sum_{j=1}^2 \hbar \nabla_k h_j(k) \mid_{\delta k = 0} \cdot \delta \vec{k} \cdot \vec{v}_j$$

if $\nabla_k h_0(k) \mid_{\delta k = 0}$ is $= 0$ and the 3 velocity vectors $\vec{v}_\mu = \nabla_k h_\mu(k) \mid_{\delta k}$ are orthogonal to $\vec{v}_\mu$ will have the form of the anisotropic (Weyl) Hamiltonian.
In 2D there are only $k_x k_y$ that we will vary so no way to find simultaneous zeros of 3 functions $h(I, \omega)$ without additional fine tuning.

$\Rightarrow$ in 2D without additional symmetry that constrains the number of independent $h(I, \omega) = 0$ the 2-bands avoid each other.

Without constraint we can only get accidental two-fold degeneracy of bands in 3D - solids.

- The dispersion $\varepsilon(k)$ is linear and similar to Weyl, e.g.

  Most important, if $h_0^{(1,2)} = 0$ or $\nu_1 = 0$ the $\mathcal{H}(\omega)$ is a 2-level system we used in the HW3D.
We then can presume that the node at \( k_0 \) is the Berry curvature of
\[
\Omega = \pm \frac{\Delta \mathbf{k}}{2|k|^2} \quad \text{where} \quad \Delta \mathbf{k} = \mathbf{k} - \mathbf{k}_0
\]
The Berry curvature field is that of a magnetic monopole with \( +' \) or \(-'\) charge.

Consider only one node or \( +'\) charge
\[
\mathcal{H}(k) = \pm \sigma \cdot \mathbf{e} \cdot (\mathbf{k}_0 - \mathbf{k}_0)
\]

**UNDER IRS**

\[
k \rightarrow -k \quad \sigma \rightarrow -\sigma \quad \mathcal{H} \rightarrow \mathcal{H} = \frac{1}{\sigma} \cdot \mathcal{e} \cdot (k + k_0)
\]

\( \Rightarrow \) Must be other node with \( k = -k_0 \) with the same charge.
Under space inversion
\[ \overline{k} \rightarrow -k \quad \text{and} \quad \sigma \rightarrow \overline{\sigma} \Rightarrow \]
\[ \mathcal{H} \Rightarrow \mathcal{H}' = \frac{1}{2} \nabla \overline{\sigma} \cdot \overline{k} + \overline{\sigma} \]

- IS requires there must be another node with \(-\overline{\sigma_0}\) with \(\overline{\sigma}\) charge.

- If both TRS and IS present
  each node will two monopoles of opposite charges \(= 0\)

**Summary**

In the absence of TRS or SI

massless lattice fermions are required
to come in pairs with opposite
helicities, or Berry charges.

Nielsen-Nielsen Theorem or fermion

doubling theorem.

Note, the net charge of all Weyl points over the BZ
must be 0.
Stability of Weyl Nodes

The stability of Weyl nodes is protected by the Gauss law: a Gaussian surface surrounding Weyl nodes detects its charge. It can only disappear if there is another opposite monopole through the surface.

To realize the Weyl semimetal, we need:

1) 3D crystal with non-degenerate bands by breaking either TRS or $\mathcal{S}$.

2) Points must be near Fermi surface where $\text{Vol} = 0$ and $V_j$ are orthogonal $\nabla \phi(k) \propto 0$. 
The Q. is now according to the bulk - surface correspondence, if W.Ss have the topo - surface states?

A:

Instead they form **SURFACE ARCS**.

Note:

If we treat \( k_2 \) as a parameter then for each value of \( k_2 \) there is a band structure which depends on \( k_x \) and \( k_y \). But if \( k_2 \neq \pm k_\) there is a gap in the band structure at F.S.
So we can define a Chern number for the system \( C(k_\pm) \).

Since \( C(k_\pm) \) is a topological index, it can change if the 2D band crossing \( k = k_\pm \). So

\[
C \left( k_- < k_\pm < k_+ \right) \neq C \text{ outside of } [k_-, k_+]
\]

Consider the case of \( C = 1 \) for

\[
k_- < k_\pm < k_+ \quad \text{and}
\]

\( C = 0 \) otherwise.

- Translational invariance in \( z \)

\( \text{finite in } x, y \) so \( k_\pm \) is a good quantum number.

\( \Rightarrow \) From the bulk - surface correspondence \( \Rightarrow \) we will have the edge states for

\[
 k_- < k_\pm < k_+ \quad \text{that intersect the Fermi surface.}
\]
Since the Fermi surface intersects an open segment in the 1D \( k_z \) space, this intersection is called the Fermi arcs.
THE END OF QM502 2020 Class
YOU ARE MY COVID-19 HEROES!

SEE NEXT PAGE
Well, I’ve been talking to you for two years and now I’m going to quit. In some ways I would like to apologize, and other ways not. I hope—in fact, I know—that two or three dozen of you have been able to follow everything with great excitement, and have had a good time with it. But I also know that “the powers of instruction are of very little efficacy except in those happy circumstances in which they are practically superfluous.” So, for the two or three dozen who have understood everything, may I say I have done nothing but shown you the things. For the others, if I have made you hate the subject, I’m sorry. I never taught elementary physics before, and I apologize. I just hope that I haven’t caused a serious trouble to you, and that you do not leave this exciting business. I hope that someone else can teach it to you in a way that doesn’t give you indigestion, and that you will find someday that, after all, it isn’t as horrible as it looks.

Finally, may I add that the main purpose of my teaching has not been to prepare you for some examination—it was not even to prepare you to serve industry or the military. I wanted most to give you some appreciation of the wonderful world and the physicist’s way of looking at it, which, I believe, is a major part of the true culture of modern times. (There are probably professors of other subjects who would object, but I believe that they are completely wrong.)

Perhaps you will not only have some appreciation of this culture; it is even possible that you may want to join in the greatest adventure that the human mind has ever begun.