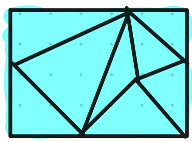
TOPOLOGY & QM

LECTURE 17

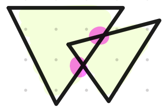
The Euler characteristic of a square

There is a rule how to partition a square into Δ pieces

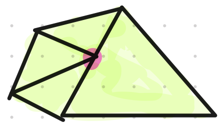


- The rule says the pieces must fit together along the edges

Bad examples:



no overlapping allowed



the vertex of a Δ cannot touch the edge of another Δ

Let's count the following elements

Δ faces	f	8
edges	e	16
verteces	v	9

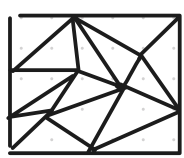
Now we calculate $f - e + v = 8 - 16 + 9 = 1$

The partioning of a figure K into Δs following the above rule is called a triangulation of K.

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

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

Problem: Calculate Euler characteristic of



Answer:

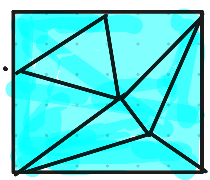
$f - e + v =$

So now you noticed does not matter how you triangulate the answer for $f(K)$ is the same.

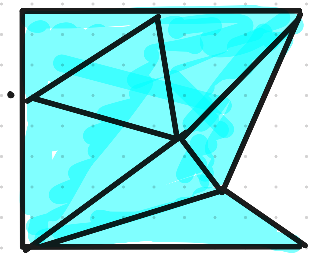
But what if we Δate the a squre into a billion of Δs? We cannot simply count it.

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

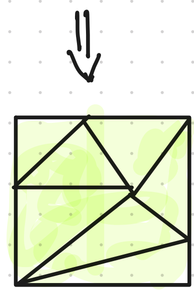
Consider any Δation



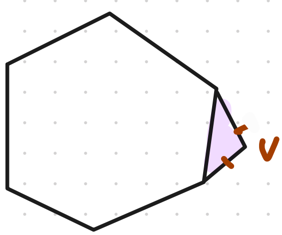
remove 1 Δ



deform it



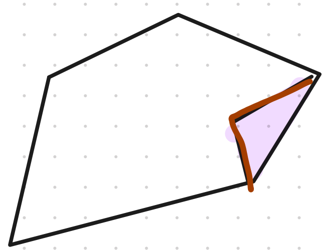
iF you observe a process of deformation You will find that we always do it by two ways:



here f, e, v change

$f \to f+1 \quad e \to e+2 \quad v \to v+1$

$f - e + v = \text{CONST}$



$f \to f+1 \quad e \to e+1 \quad v \to v$

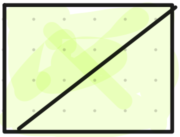
$f - e + v = \text{CONST}$

But in both cases

$f - e + v$ is constant!

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

$f = 2$
$e = 5$
$v = 4$

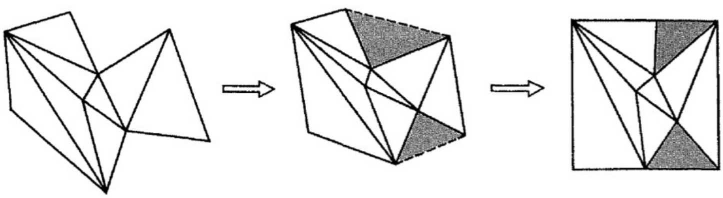


$f - e + v = 1$

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

Proof:
After we triangulate a polygon we can add a Δ and deform the resulting figures to a $\square$.



add shaded triangles

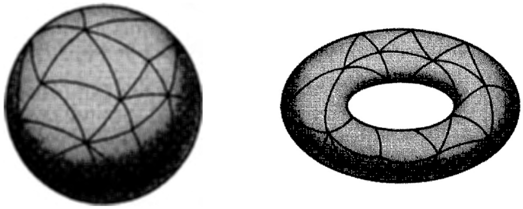
$f \to f + 2$
$e \to e + 2$
$v \to v$

$$\boxed{\chi(\square) = 1}$$

Next we switch to other surfaces:

Sphere and torus

Now we can make a patch work on the surface of torus or sphere to produce a similar triangulation.

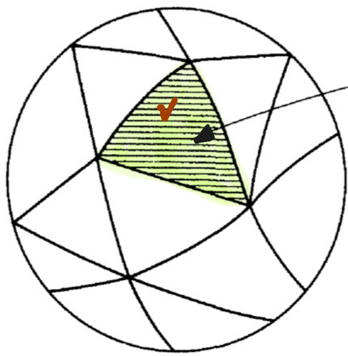


What is χ(sphere) and χ(torus)?

Theorem: χ(sphere) = 2 and χ(torus) = 0

I only prove it for a sphere.

Consider a Δation of the sphere and let's remov 1 Δ.



Since the sphere with minus one Δ can be stretched to the plane. This figure is equal to the Large triange with χ(polygon) = 1

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

$$\chi(\text{sphere}) = \chi(\underbrace{\text{sphere} - \Delta}_{\text{polygon} \equiv 1}) + 1 = 2$$

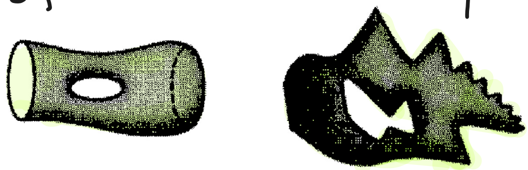
EOP

CLOSED SURFACE

in topology we consider 2 figs to be different if we cannot transform those via elastic deformations.

But what if a figure has holes?

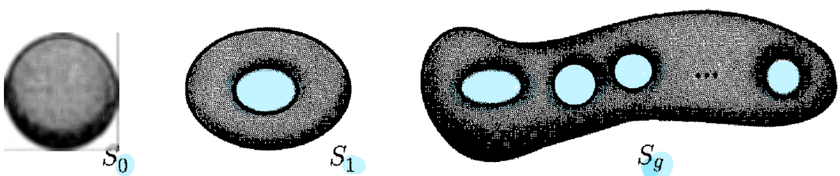
Example of non-closed surfaces:



(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:

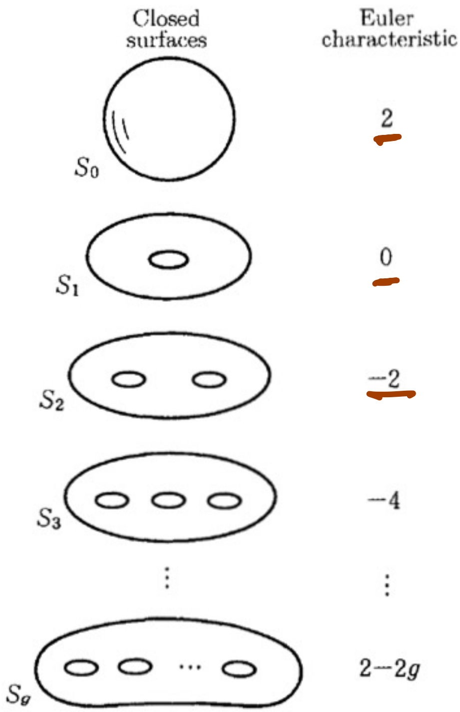
$\chi(S_0) = 2 \quad \chi(S_1) = 0$, so what's $\chi(S_g)$?

I'm going to skip the proof but here is the theorem:

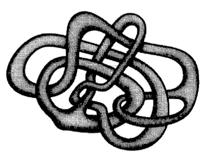
$$\boxed{\chi = 2 - 2g}$$

for a surface with a boundary b: $\chi = 2 - 2g - b$

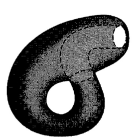
Let's test this formula:



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



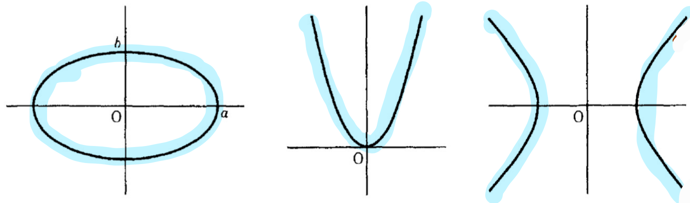
2) What is genus of this figure (Klein bottle)?



CURVATURE OF SURFACE

GAUSSIAN CHARACTERISTICS

Q: Is there any connection between $\chi(S_g)$ and local curvature of a surface?

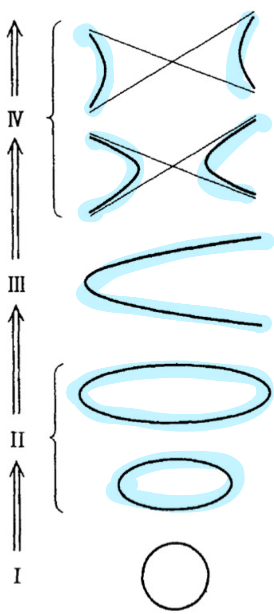


Ellipse Parabola Hyperbola

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}=1 \qquad y=ax^2 \qquad \frac{x^2}{a^2}-\frac{y^2}{b^2}=1$$

a and b > 0   a, b > 0

those 3 figures a called conic sections

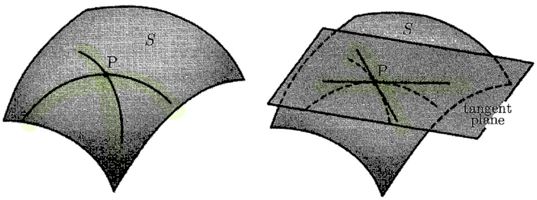


Flow chart of intersections of a double cone and a plane from various positions

← the reason we call it conical b/c those are cross-sections of a cone by a plane

How to quantify curvature?

① Tangent Plane

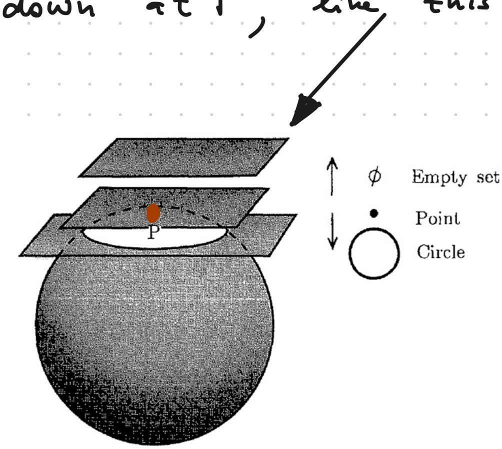


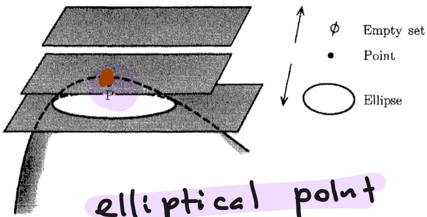
The protocol is simple

- 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 poin P
- Draw a plane which includes P and 2 tangent lines. This plane is called the tangent plane.

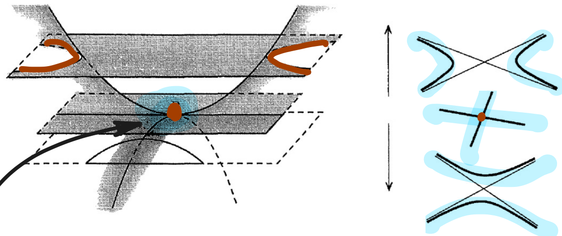
- The way to observe the curvature of the surface S is to shift this plane up and down at P, like this:





elliptical point

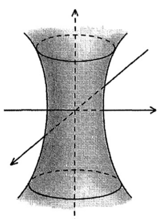
For the convex surface the result is the same.



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

hyperbolic curving or hyperbolic point

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!

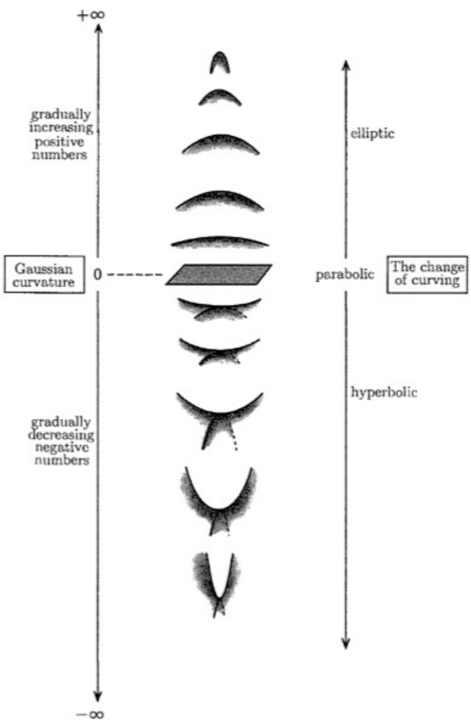
Consider a ball made of clay. Every point on the surface of the ball is an elliptic point. But if we press it with our fingers and make an indentation, then hyperbolic points appear on the indented region of the surface. In this process of changing from convexity to concavity, parabolic curving appears 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

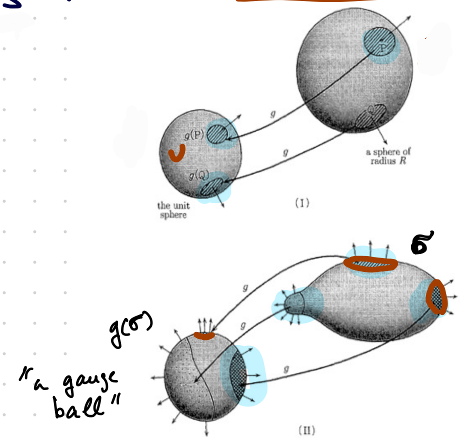
elliptic $\longrightarrow$ parabolic $\rightarrow$ hyperbolic?

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

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



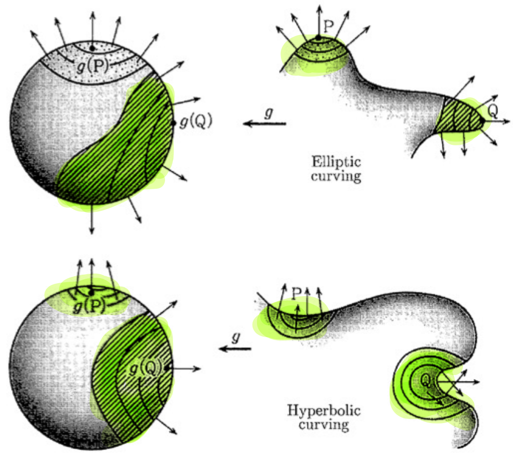
$$\boxed{K(P) = \lim_{\sigma \to P} \frac{\text{area of } g(\sigma)}{\text{area of } \sigma}}$$

Gauss - Bonnet theorem

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

$$K(P) = \underline{1/R^2}$$

▷ To arrive at this conclusion we map the sphere to the unit sphere by the transformation with a similarity ratio $= \underline{\frac{1}{R^2}}$ $\left[\frac{\cancel{4\pi} r^2 = 1}{\cancel{4\pi} R^2} = \frac{1}{R^2} \right]$



In general

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

two most extremes

Intuitive picture of a gaussian mapping

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

▷ 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 - Bonnett 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 $K(P)$ over a surface is equal to the Euler characteristic χ of the surface $\times 2\pi$

$$\frac{1}{2\pi} \cdot \int_S K(P)\, d\sigma = \chi(S)$$

▷ We will not prove the theorem, but let's verify it on a sphere $K(P) = 1/R^2$:

$$\frac{1}{2\pi}\int_S K(P)\,d\sigma = \frac{1}{2\pi}\cdot\frac{1}{R^2}\cdot\underbrace{\int_S d\sigma}_{\text{surface of a sphere}} = \frac{1}{2\pi}\cdot\frac{1}{R^2}\cdot 4\pi R^2 = 2\,!$$

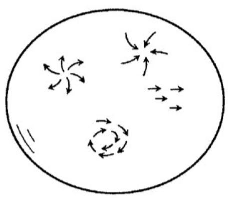
Recall $\chi(S_0) = 2$

▷ The fundamental result:

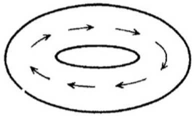
$$\boxed{\frac{1}{2\pi}\int_S K(P)\,d\sigma = \chi(S_g) = 2-2g}$$

!

Vector Fields on Surface



Here is the wind blowing on the sphere



The same on torus

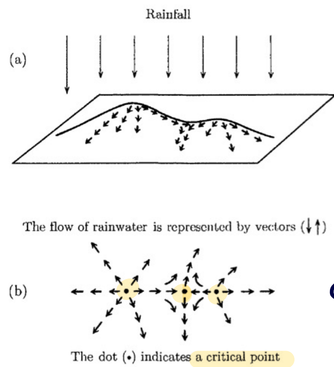
Q: What's the difference?

BTW: if we have a surface described by the parametric $S(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix} \Rightarrow \boxed{K = \frac{x'(t)\,y''(t) - y'(t)\,x''(t)}{(x'(t)^2 + y'(t)^2)^{3/2}}}$

▷ Imagine that the surface is a field with alternating regions of concavity and convexity and with small vectors in them.

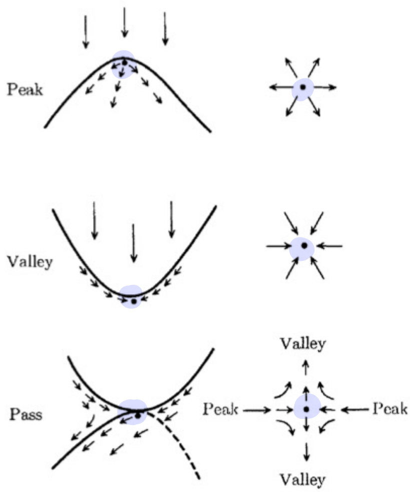
▷ The places where flow stops is called a critical point.

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



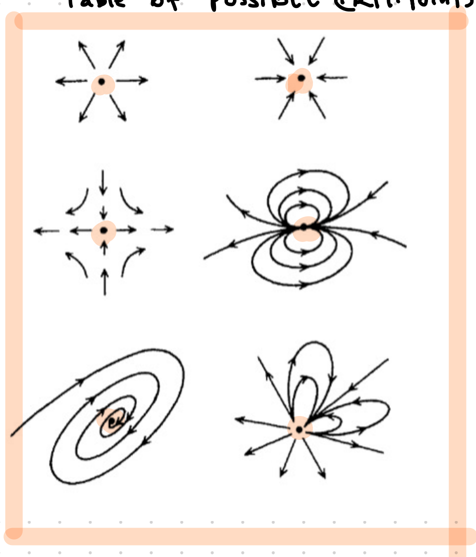
critical points.

Check this figure:



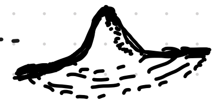
▷ If you spend enough time you can descover that the only critical points are:

Table of POSSIBLE CRIT. Points



▷ Let's introduce a new tool: **the index of a critical point**

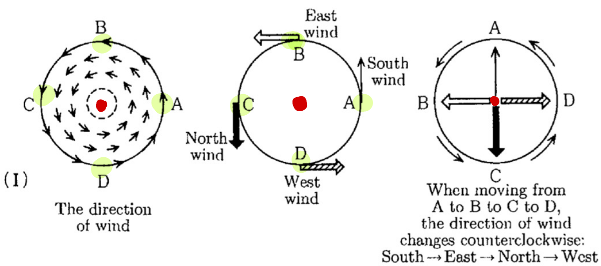
e.g. if the top of a mountain is as flat as the top of a table, the fallen rain will collect on those flat areas. In such a case the critical points are everywhere.



▷ Now think of a flow of H_2O 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.

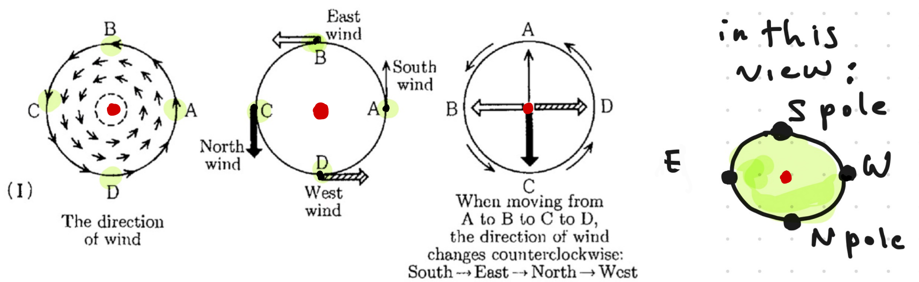
▷ Move around the path and measure the direction of the flow at each point



▷ Since the wind directions revolve once around the circle counter-clockwise we assing the index $P = +1$

Let us discuss the way you get 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 wall always counterclockwize
   A → B → C → D → A

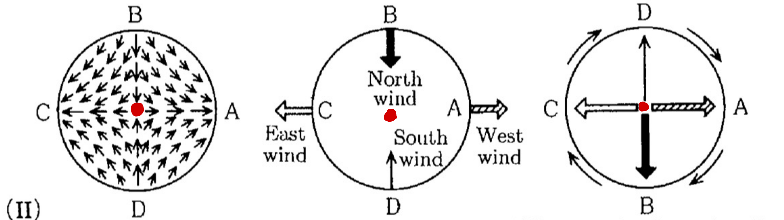
2. Determine the direction of the vector field at each of the point A ↑, B ←, C ↓, D → etc.

3. Bring those vector to the special poin whose index you try to define.

! The position of the points on the countour will change, e.g. in our case A → B, B → C, C → D and D → A

4. Observe the direction and the number of times you have to move around A → B .... → A
   This number and its sing is your index, i (P).

▷ What about the critical point index here?



When moving from A to B to C to D, the direction of wind changes clockwise: West → North → East → South

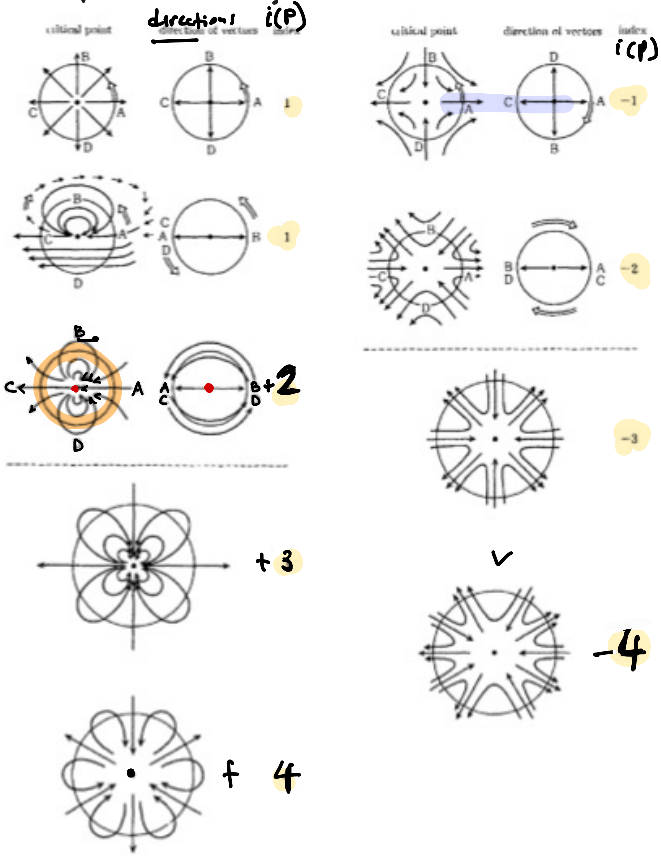
$i(P) = -1$

▷ General protocol: Draw a circle around a critical point P, and go around counter clockwize, observe change in the direction of a vector.

If the direction of the vector revolves n times we say $i(P) = +n$
Otherwize $i(P) = -n$

Next page figure shows few interesting examples:

Examples of critial points and their indeces.



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 indeces $i(P)$ is equal to the Euler characteristic of S_g

$$\chi(S_g) = 2 - 2g$$

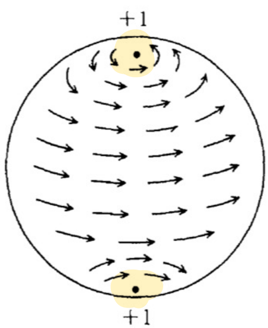
$$\boxed{\sum i(P) = 2 - 2g}$$

▷ Few comments are due:

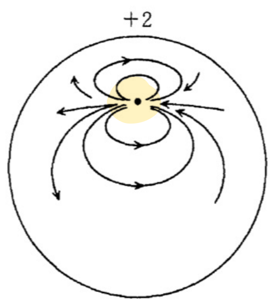
if the surface is a sphere then $\chi(S_0)=2$

What can we say about the surface?

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



The flow of west winds



▷ Consider another example

a dipolar magnetic monopole on the surface of the sphere.

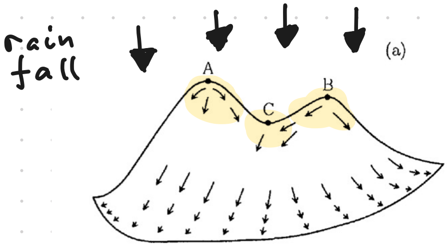
The critical index of this point is $i(P) = +2$

it means that's the only one critical point for this kind of vector field.

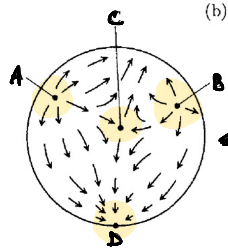
Or there can be only ONE dipole magnetic monopole on Earth!

Now you can try to search for it.

▷ Here is another example of a "sphere"



The flow of water stops at the base of the mountain



Point D where the base of the mountain has been gathered up

what's $\Sigma i = ?$

This vector field has 4 critical points:

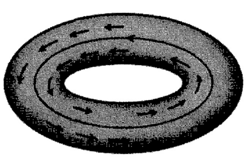
- 2 at peaks A & B $\quad i(A) = i(B) = +1$
- at pass C $\quad i(C) = -1$
- point D where water gathers $\quad i(D) = +1$

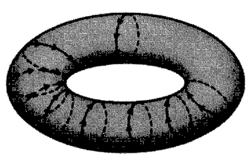
The sum of the indexes $\sum i(A, B, C, D) = +1 +1 -1 +1 = +2$

$\chi(S_0) = 2$ as well.

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

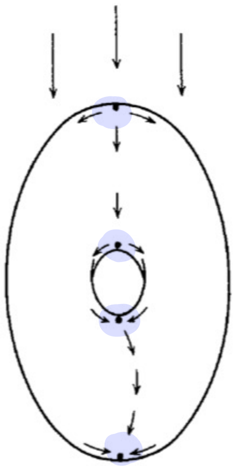
This means that there is a vector field with no critical points or ALL critical point indeces can be only compensated ones so their sum is zero!





Field with no critical points!

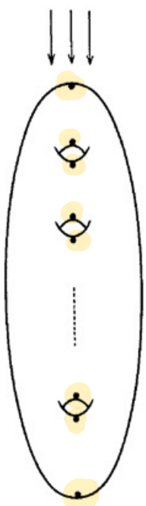
But what if the rainfall vector field drops on the torus



	index
	1
	-1
	-1
	1
sum	0

Again we have 4 critical points

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



critical point	index
• peak	1
• saddle	-1
• saddle	-1
• saddle	-1
• saddle	-1
• saddle	-1
• saddle	-1
• valley	1
the sum of indices of critical points	$2-2g$

SUMMARY

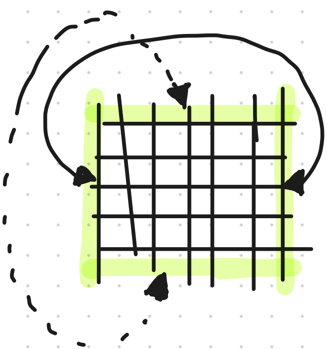
$$\chi(S_g) = 2 - 2g = \sum_{S_g} i(P) =$$
$$= \frac{1}{2\pi} \cdot \oint_S K(P)\, d\sigma$$

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

i = singularity in $E(\bar{k})$ dispersion

$K(P)$ = curvature = Berry potential

$g = 1$ = because of the periodic boundary conditions



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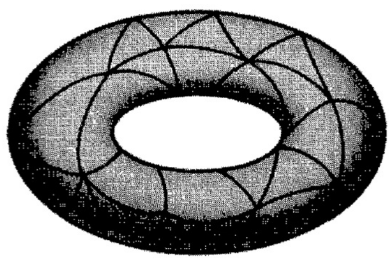


$\chi(S_1) =$
$= 0$

BERRY PHASE and all that

So far in our discussion we had a missing factor called φ - phase of the $|\psi\rangle$ function.

$$|\psi\rangle \to |\tilde{\psi}\rangle = e^{i\varphi}|\psi\rangle \Rightarrow \langle\psi|\hat{O}|\psi\rangle = \\ = \langle\tilde{\psi}|\hat{O}|\tilde{\psi}\rangle$$

This works b/c $\hat{O}$ doesn't act on φ which is just a number of magnitude 1.

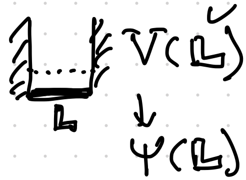
- But there are some observables which are NOT expectation values of the operator $\hat{O}$ and this arbitrary phase plays the role of an observable.

This happens when our hamiltonian H has a parametric dependence.

In this case φ is called a geometric phase which describes how the wave. f. depends on the parameters related to geometric features of the system.

! In a trully isolated system there is no Berry phase. !

BERRY PHASE and all that



definition:

$$\hat{H}(\vec{q})\,|\Psi_{\underline{q}}\rangle = \epsilon_q\,|\Psi_q\rangle$$

q is a some parameter

When solving the Shr. eqn φ appears in the form $e^{i\varphi}$ for the ground state solution.

Note: if we deal with analytical solution
$\varphi = 0$
if numerical often used φ - a random number.

Suppose we have 2 different ground states for q_1 with the phase φ_1
q_2 φ_2

And let's try to explicitely remove the phase φ for each ground state

i.e. $|\Psi_{g_1}\rangle \rightarrow |\tilde{\Psi}_{g_1}\rangle = e^{-i\varphi_1}\,|\Psi_{g_1}\rangle$

$|\Psi_{g_2}\rangle \rightarrow |\tilde{\Psi}_{g_2}\rangle = e^{-i\varphi_2}\,|\Psi_{g_2}\rangle$

this is known as choosing a gauge

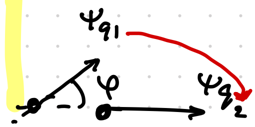
The overlap of the two phase-corrected functions

$$\langle\tilde{\Psi}_{g_1}|\tilde{\Psi}_{g_2}\rangle = e^{i(\varphi_1 - \varphi_2)}\langle\Psi_{g_1}|\Psi_{g_2}\rangle$$

BERRY PHASE and all that

But since we agreed to remove all the phase dependence the left side must be only the magnitude $|\langle\Psi_{q_1}|\Psi_{q_2}\rangle|$ of the overlap which allows us to define the relative phase $\Delta\varphi_{12}$ as:

$$e^{-i\varphi_{12}} = \frac{\langle \overset{H(q_1)}{\Psi_{q_1}} | \overset{H(q_2)}{\Psi_{q_2}} \rangle}{|\langle \Psi_{q_1} | \Psi_{q_2} \rangle|}$$



STOP!

or $\quad \ln e^{-i\Delta\varphi_{12}} = \ln(\ldots)$

$$-i\Delta\varphi_{12} = \ln(\ldots) \quad \text{or}$$

$$\Delta\varphi_{12} = -\operatorname{Im}\left[\ln \frac{\langle\Psi_{q_1}|\Psi_{q_2}\rangle}{|\langle\Psi_{q_1}|\Psi_{q_2}\rangle|}\right]$$

Now lets consider a small difference in $q_1 \to q_2$ $= \Delta q$

$q_2 = q_1 + \Delta q \to 0$

$$e^{-i\Delta\varphi_{12}} = \frac{\langle\Psi_q|\Psi_{q+\Delta q}\rangle}{|\langle\Psi_q|\Psi_{q+\Delta q}\rangle|}$$

$|\Psi_{q+\Delta q}\rangle \cong |\Psi_q\rangle + \nabla_q|\Psi_q\rangle\cdot\Delta q + \ldots$

$$\cancel{1} - i\Delta\varphi_{12} \cong \langle\Psi_q|\nabla_q|\Psi_q\rangle\cdot\Delta q + \cancel{\overset{=1}{\langle\Psi_q|\Psi_q\rangle}}$$

$$-i\Delta\varphi_{12} \simeq \langle\Psi_q|\nabla\Psi_q\rangle\cdot\Delta q \Rightarrow \boxed{d\varphi = i\langle\Psi_q|\nabla\Psi_q\rangle}$$

BERRY PHASE and all that

And now we can calculate Berry phase

$$\boxed{\gamma = \oint d\varphi = i \oint \langle \psi_q | \nabla_q \psi_q \rangle \cdot d\bar{q}}$$

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

localy

Let's verify this:

$$|\tilde{\psi}_q\rangle = e^{-i\varphi(q)} |\psi_q\rangle$$

$$\nabla_q |\tilde{\psi}_q\rangle = [-i \nabla_q \varphi(q)] \underbrace{e^{-i\varphi(q)} |\psi_q\rangle}_{|\tilde{\psi}_q\rangle} +$$

$$+ \; e^{i\varphi(q)} [\nabla_q |\psi_q\rangle]$$

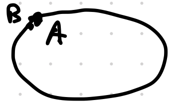
now the B.p. is:

$-i \times i$

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

$$i\oint \langle \tilde{\psi}_q | e^{-i\varphi(q)} \nabla_q |\psi_q\rangle dq + (-i \times i) \oint \nabla_q \varphi(q) \cdot dq =$$

BERRY PHASE and all that



recall:

$$\oint \underline{\nabla_q \varphi(q)} \cdot dq = \varphi(A) - \varphi(B) \overset{A=B}{=} 0$$

Returning to the original value of $\tilde{\gamma}$:

$$\tilde{\gamma} = i \oint_c \langle \tilde{\psi}_q | e^{-i\varphi(q)} \nabla_q | \psi_q \rangle =$$

$$\langle \tilde{\psi}_q | = \langle \psi_q | e^{+i\varphi(q)}$$

$\Rightarrow$

$$= i \oint_c \langle \psi_q | \cancel{e^{i\varphi(q)}} \, \cancel{e^{-i\varphi(q)}} \nabla_q | \psi_q \rangle dq =$$

$$= i \oint_c \langle \psi_q | \nabla_q | \psi_q \rangle dq = \gamma$$

EOP

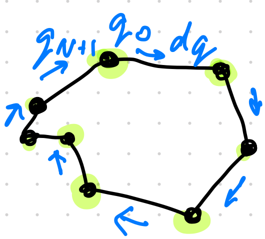
γ or B. ph. is locally phase invariant and as such is observable.

BERRY PHASE and all that

ANOTHER LOOK AT GAUGE INVARIANCE

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

$$\Delta \varphi_{12} = -\mathrm{Im}\left[\ln\left(\langle \psi_{q_1} | \psi_{q_2} \rangle \right) \right]$$



here $q_0 = q_{N+1}$

and $q_{i+1} = q_i + dq$

Then we can write down

$$\boxed{\Delta \varphi} = -\mathrm{Im}\left[\sum_{i=0}^{N} \ln\left(\langle \psi_{q_i} | \psi_{q_{i+1}} \rangle \right) \right] =$$

$= \quad \sum \ln = \ln \prod$

$$= \boxed{-\mathrm{Im}\left[\ln\left(\prod_{i=0}^{N} \langle \psi_{q_i} | \psi_{q_{i+1}} \rangle \right) \right]}$$

BERRY PHASE and all that

But is the descrete B.p. locally gauge invariant?

To check we introduce

$$|\tilde{\psi}_q\rangle = e^{-i\varphi(q)}|\psi_q\rangle$$

Consider $\prod \langle \tilde{\psi}_{q_i} | \tilde{\psi}_{q_{i+1}} \rangle \equiv \langle q_0 \underbrace{|q_1\rangle\langle q_1|}_{e^{i\varphi(q_1)} \cdot e^{-i\varphi(q_1)} = 1} q_2\rangle \cdot \ldots \cdot \langle q_N | q_{N+1} \rangle$

So the phases cancel out betwen the successive steps b/c they arize from bra and ket with the same index and for q_0 and q_{N+1} phase is also the same. as they represent the same end point.

- I want to stress only $\prod$ or $\oint_c$ is locally gauge invariant the integrand itself NOT!

- The value of γ depends on the countour of integration.

Now I want to consider a very special case: when the parameter q is REAL

BERRY PHASE and all that

if this is the case we can introduce two quantities:

Berry connection

$$\boxed{\bar{A}(\bar{q}) = i \langle \psi_q | \bar{\nabla}_q \psi_q \rangle} \longrightarrow \text{a 3-component vector}$$

Berry curvature

and $$\boxed{\Omega_{\alpha\beta}(q) = \frac{\partial A_\beta(\bar{q})}{\partial q_\alpha} - \frac{\partial A_\alpha(q)}{\partial q_\beta}}$$

ANTISYMMETRIC TENSOR OF 2^d rank

$$= i \left[\left\langle \frac{\partial \psi_q}{\partial q_\alpha} \middle| \frac{\partial \psi_q}{\partial q_\beta} \right\rangle - \left\langle \frac{\partial \psi_q}{\partial q_\beta} \middle| \frac{\partial \psi_q}{\partial q_\alpha} \right\rangle \right] =$$

B/c q is real

$$= -2\, \mathrm{Im} \left\langle \frac{\partial \psi_q}{\partial q_\alpha} \middle| \frac{\partial \psi_q}{\partial q_\beta} \right\rangle$$

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

by the cyclic permutation of indeces

e.g. $\Omega_{xy} \longrightarrow z$ component of $\vec{\Omega}$

or $\Omega_{\alpha\beta} = \epsilon_{\alpha\beta\gamma} \Omega_\gamma$ the Levi-Civita tensor

BERRY PHASE and all that

Thus now I can write down $\vec{\Omega}$ as the curl of A

$$\left[\Omega_{\alpha\beta}(q) = \frac{\partial A_\beta(q)}{\partial q_\alpha} - \frac{\partial A_\alpha(q)}{\partial q_\beta} \right]$$

$$\boxed{\vec{\Omega}(\vec{q}) = \nabla_q \times A(q)}$$

And finally:

Berry connection or Berry potential

$$\boxed{\text{Berry phase} \quad \gamma = \oint_C A(\bar{q})\cdot d\bar{q} = \oiint_S \nabla_q \times A(q) \cdot d\bar{S} \doteq \underline{i\oint \langle \psi_q | \nabla_q \psi_q \rangle dq} = \oiint_S \bar{\Omega}(\bar{q}) \cdot d\bar{S}}$$

Berry curvature

here S is the surface enclosed by C and $d\bar{S}$. The surface unit vector points in the right hand rule direction.

To connect you to the perturbation theory I can show how to calculate γ from the perturbation theory. i.e if $\psi_q^{(0)}$ $E_q^{(0)}$ is ground state and

BERRY PHASE and all that

$\psi_q^{(n)}$ and $\epsilon_q^{(n)}$ is the excited state

we have $\left|\frac{\partial \psi^{(0)}}{\partial q_\alpha}\right> = \sum_{n=0} |\psi^{(n)}>$.

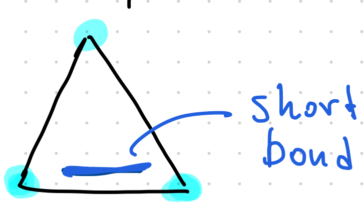
$$\cdot \frac{<\psi_q^{n}| \partial \mathcal{H}_q / \partial q_\alpha | \psi_q^{(0)}>}{\epsilon_q^{(0)} - \epsilon_q^{(n)}}$$ and

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

$$= -2\, \mathrm{Im}\left[\sum_{n=0} \frac{<\psi_q^{(0)}| \partial H_q / \partial q_\alpha | \psi_q^{(n)}><\psi_q^{(n)}| \frac{\partial H_q}{\partial q_\beta}| \psi_q^{(0)}>}{(\epsilon_q^{(0)} - \epsilon_q^{(n)})}\right]$$

The advantage, we don't need to calculate derivatives of $\psi_q^{(n)}$ but only $\mathcal{H}_q$. But you need to sum up over all $|\psi_q^{(n)}>$

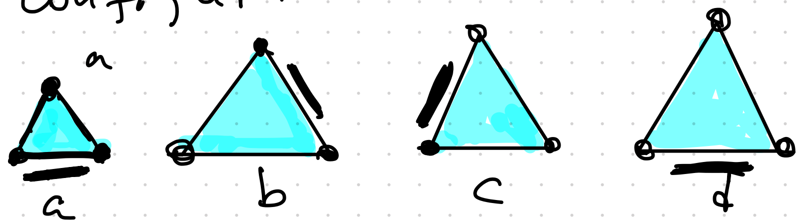
For fun let's calculate B. ph. of a molecule, or a triangular lattice solid.



BERRY PHASE and all that

EXAMPLE I

Thus we have several configurations:



$a = d$

recall $\gamma = -\mathrm{Im}\ln \prod_{0}^{N} \langle \psi_i | \psi_{i+1} \rangle$

in the 3-atomic molecule the states are:

$$|\psi_a\rangle = |\psi_d\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |\psi_b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{2\pi i/3} \end{pmatrix}$$

$$|\psi_c\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{4/3\pi i} \end{pmatrix} \Rightarrow$$

$$\gamma = -\mathrm{Im}\ln\left[\langle \psi_a | \psi_b \rangle \langle \psi_b | \psi_c \rangle \langle \psi_c | \psi_d \rangle\right]$$

$$= -\mathrm{Im}\ln\left[\left(\frac{e^{\pi i/3}}{2}\right)^3\right] = -\pi$$

So $\underline{\gamma = -\pi}$.

And the Chern index is $C = \left|\frac{\gamma}{2\pi}\right| = \frac{1}{2}$

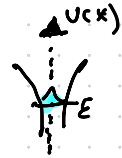
More on Chern number follows later.

BERRY PHASE and all that

Example 2

Aharonov - Bohm effect as a Berry phase

Our q.m. system is made of an electron and the potential $V(r)$ which localizes it.



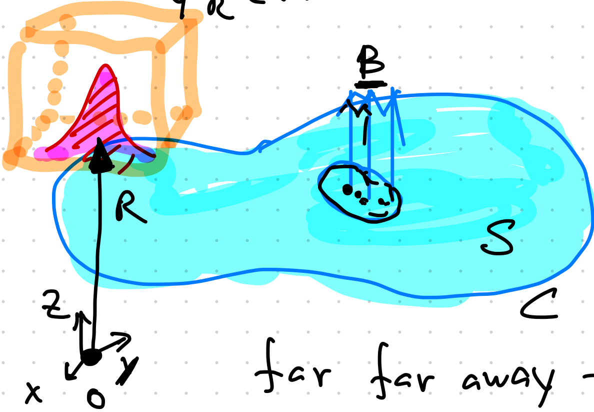
$$\mathcal{H}\,\psi(r) = \left[-\frac{\hbar^2}{2m_e}\nabla_r^2 + V(r) \right] \psi(r) = \epsilon\,\psi(r)$$

Imagine we shift the origin of the confining potential by $\bar{R}$ so the hamiltonian is $\bar{R}$-parameter dependent

$$\hat{\mathcal{H}}_R\, \psi_R(r) = \left[-\frac{\hbar^2 \nabla_r^2}{2m_e} + V(r - R) \right] \psi_R(r) = \epsilon_R\, \psi_R(r)$$

translational invarvance requires:

$$\psi_R(r) = \psi(r - R) \qquad \epsilon_R = \epsilon$$



Now I will transport the electron ψ_R around a closed path C which is far far away from the region with magnetic field.

BERRY PHASE and all that

The new hamiltonian is now

$\mathcal{A}$ ← Berry connection

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

← vector potential

$B = \nabla_r \times A(r)$

The new w.f. for this hamiltonian

$$\Psi_R(r) = e^{-\frac{ie}{\hbar c}\int_R^r A(r')\cdot dr'} \cdot \varphi(r-R)$$

$R=q$

$\frac{e^{i\varphi(q)}|\Psi_q\rangle}{}$

with the phase $\varphi_R(r) \equiv -\frac{e}{\hbar c}\int_R^r A(r')\cdot dr'$

which depends on PATH and is not well defined!
Let's try to restore the single 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:

$$\mathcal{A}(R) = i\langle\Psi_R|\nabla_R\Psi_R\rangle = \frac{-e}{\hbar c}A(R) +$$

$$i\int \varphi^*(\underbrace{r-R}_{r'})\nabla_R\,\varphi(r-R)\cdot dr \;\rightarrow\; \text{it is } =0 \xrightarrow[\text{prove}]{\text{to}}$$

BERRY PHASE and all that

First I define $r' \equiv r - R$ and use the chain rule to swith the variables:

$$\int \psi^*(r') \nabla_{r'} \psi(r') \cdot dr' \left(\frac{\partial r'}{\partial R}\right) = \underset{\frac{\partial R'}{\partial R}}{-} \underline{\int \psi^*(r') \nabla_{r'} \psi(r') dr'} =$$

~ expectation value of momentum in $\psi(r')$ which is for a bound state = 0

$$= \emptyset$$

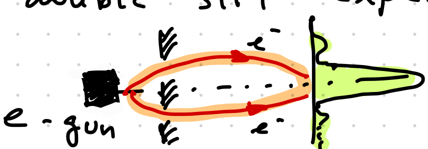
What remains is to calculate the B. P.

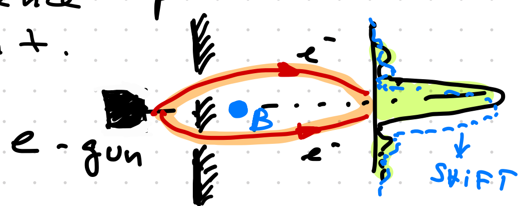
$$\gamma = -\frac{e}{\hbar c} \oint_c A(R)\, dR \overset{\text{stoke's theorem}}{=} -\frac{e}{\hbar c} \oiint_S (\nabla_r \times A(r)) \cdot dS$$

$$= -\frac{e}{\hbar c} \iint_S \bar{B} \cdot d\bar{S} = -2\pi \frac{\phi}{\Phi_0}$$

$\Phi_0 = \hbar c / e \equiv$ FLUX QUANTUM 2.067833×10^{-15} Wb

In other words $\gamma \sim \phi$ of the $\bar{B}$.
B.p. is sampling the single "dot" region of B and is sensed by $|\psi\rangle$ transported around this point. This phase was measured in the change of the inteference 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 Φ at $r=0$.

We punched a hole in the manyfold!

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, $\pi_1(S^1) = \mathbb{Z}$

This mapping is characterized by by an integer winding number. {or integer critical index $i(P)$}

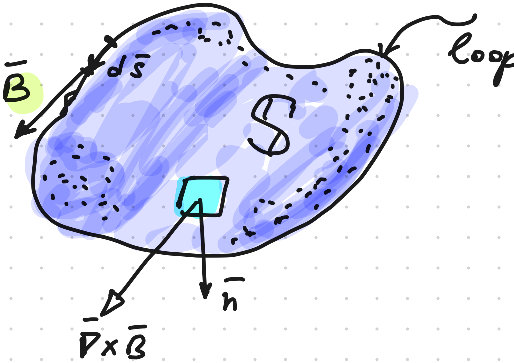
Geometrical phases only exist when the space is NOT simply connected.

② Note if the ground state $|\psi_g\rangle$ is N-degenerate we need to use NON-ABELIAN Berry connection.

SUMMARY OF A-B.

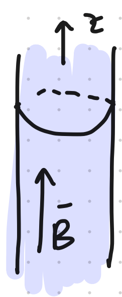
▷ Recall in magnetostatics:

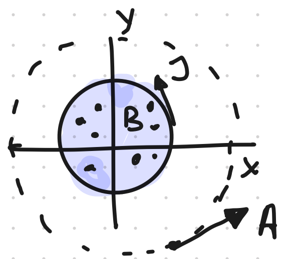
$$\oint \bar{B}\cdot d\bar{s} = \iint \underbrace{(\nabla \times \bar{B})}\cdot \bar{n}\, dS$$



▷ and also we can write

$$B = \bar{\nabla} \times \bar{A}$$





$B_x = B_y = 0$

$B_z \neq 0$

$A_x \neq 0$

$A_y \neq 0$

$$\oint \bar{A}\cdot d\bar{s} = B\cdot \pi r^2 = \text{FLUX}$$

Topology	Magnetism	Quantum
Gaussian curv. K(P)	$\nabla \times B$	Berry curvature $\bar{\nabla} \times \langle u \| \bar{\nabla}_\lambda \| u \rangle$
Total curvature Genus 2 − 2g Σ crit. indeces	FLUX OF B Through S	Berry phase

▷ Berry etc.

$$\oint_\lambda \underbrace{\langle u_\lambda | \nabla_\lambda | u_\lambda \rangle}_{\equiv A(\lambda)\ \equiv\ \text{Berry potential}} d\lambda \equiv \oint \bar{A}(\lambda)\cdot d\bar{\lambda} \equiv \iint_S \underbrace{\bar{\nabla}\times A}_{\equiv\ \text{Berry curvature}}\, ds$$

Berry phase $\varphi = -\mathrm{Im}\left(\text{total Berry curvature}\right)$

also $\oint \bar{A}(\lambda)\, ds$ = FLUX OF BERRY CURVATURE

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

$\equiv$ 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 e^- is described by a periodic (Bloch) w.f $\boxed{\psi_k^{(n)}(r) = e^{ik\cdot r} \cdot U_k^{(n)}(r)}$

$$|U_k^{(n)}(r)\rangle = |U_k^n(\bar{r} + n\bar{a})\rangle$$

n - is a band index

The hamiltonian is

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

and later we will add an electric field as perturbation.

Recap $\mathcal{A}^n(k) = i\langle U_k^{(n)}|\nabla_k U_k^{(n)}\rangle \Rightarrow$

$$\Omega_{\alpha\beta}^{(n)}(k) = i\left[\left\langle\frac{\partial U_k^{(n)}}{\partial k_\alpha}\middle|\frac{\partial U_k^{(n)}}{\partial k_\beta}\right\rangle - \left\langle\frac{\partial U_k^{(n)}}{\partial k_\beta}\middle|\frac{\partial U_k^{(n)}}{\partial k_\alpha}\right\rangle\right]$$

$$\vec{\Omega}^n(k) = i\langle\nabla_k U_k^{(n)}| \times |\nabla k_k^{(n)}\rangle$$

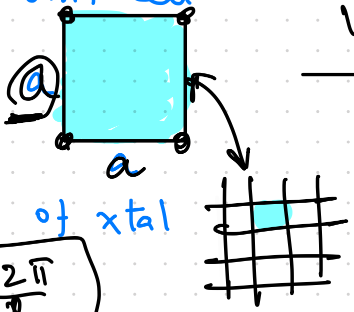
and $$\gamma^{(n)} = i\oint_C \langle U_k^{(n)}|\nabla_k U_k^{(n)}\rangle \cdot d\bar{k}$$

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

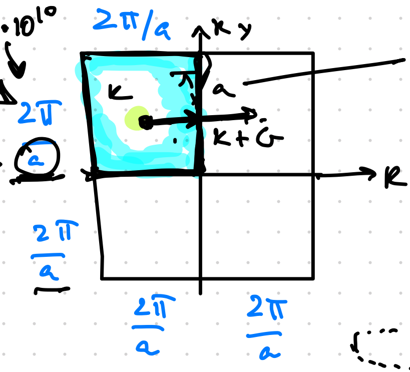
and the path is realize by moving a point k to the $k + G = 2\pi/a$

→ real space unit cell of xtal

$|\mathring{A}|$ @

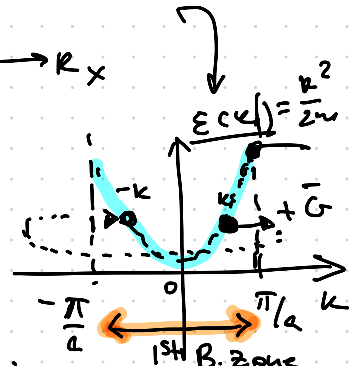


$V \to 2\pi/a$



$|G| = \pi/a$

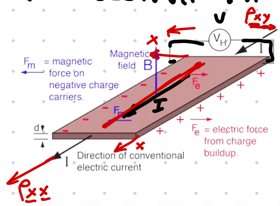
$\boxed{K = \frac{2\pi}{\lambda}}$



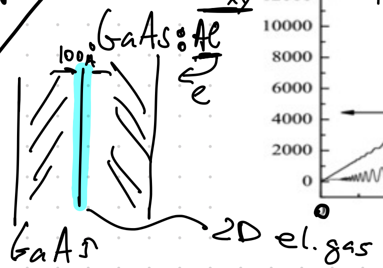
Thus $\bar{k} \to \bar{k} + \bar{G}$ transport loops the electron within the same B.Z.

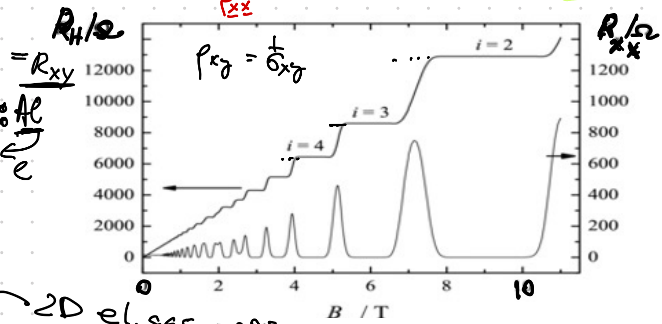
Now lets place the electron into the field

QUANTUM HALL EFFECT

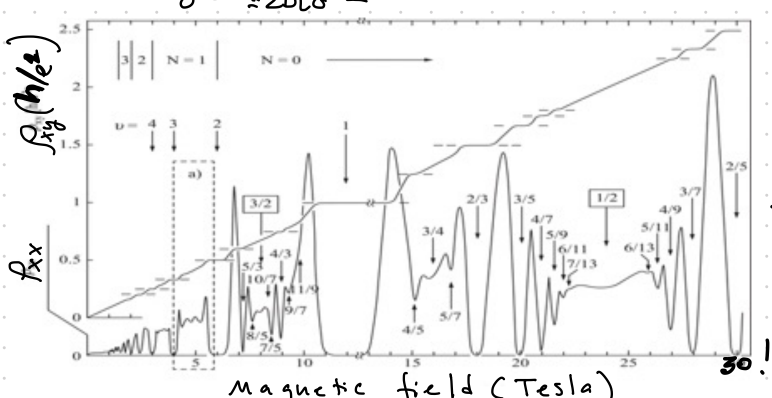


EXPERIMENTAL





Integer Quantum Hall effect = IQHE



Fractional quantum Hall effect = FQHE

Topological properties of IQHE

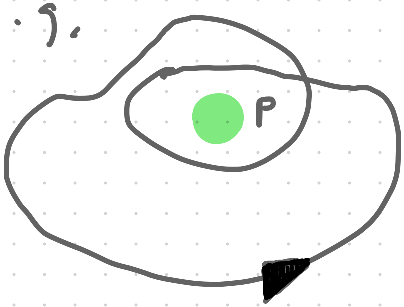
Global
$\checkmark$ Geometrical properties of an object in the mathematical space.

e.g. K-space for the electron in the Hilbert space.

The goal is to classify objects based on geometrical properties:

- bending, stretching ok
- ✗ poking holes and glueing is NOT!

e.g.



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

"Answer: 2 times".

Lets try this mathematically:

1.st we define the function

$z(t)$, $t \in [0,1]$, $t \in \mathbb{R}$

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

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

Now we can define the integral!

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

Lets confirm the Q_I is the quantity we want:

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

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

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

$$= [\varphi(1) - \varphi(0)]/2\pi$$

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

Most important we classify all possible paths in 2D:

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

Lets 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 $\psi_{nk}(x) = U_{nk}(x) e^{ikx}$

n - band index

k - wave vector

2) Apply 1^{st} order perturbation theory in the weak electric field $\bar{E} = E_x \cdot \bar{e}_x$

the electric potential $(B=0)$

$$\phi_{el}(x) = eE_x \cdot x = \underbrace{-i\frac{d}{dk_x}} \cdot eE_x$$

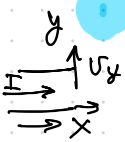
The perturbed w.f.

$$|n\rangle = |n_0\rangle - \sum_{m_0 \neq n_0} \frac{|m_0\rangle\langle m_0| ie E_x \cdot \frac{d}{dk_x}|n_0\rangle}{E_{n_0} - E_{m_0}}$$

E_{n0} E_{m0}

$|n_0\rangle$ and $|m_0\rangle$ solutions of unperturbed hamiltonian:

Lets determine the velocity in $\bar{y}$-direction



$v_y = \langle n | \hat{v}_y | n \rangle = \langle n_0 | v_y | n_0 \rangle \to 0$ $-$

$$- ie E_x \cdot \sum_{m_0 \neq n_0} \frac{\langle n_0 | v_y | m_0 \rangle \langle m_0 | \frac{d}{dk_x} | n_0 \rangle}{E_{n_0} - E_{m_0}} + h.c.$$

$\rho_{xy} = \frac{1}{\sigma_{xy}} = ?$

integer?

$$v_y = dy/dt = -\frac{i}{\hbar}[\hat{H}, y] \leftarrow$$ verify from $i\hbar \frac{\partial \psi}{\partial t} = H\psi$

$$\langle n_0 | v_y | m_0 \rangle = -\frac{i}{\hbar}\left(\langle n_0 | Hy | m_0 \rangle - \langle n_0 | yH | m_0 \rangle \right)$$

$$= -\frac{i}{\hbar} \langle n_0 | y | m_0 \rangle \cdot (E_{n_0} - E_{m_0})$$

$$y = -i \frac{\partial}{\partial k_y}$$

$$\langle n_0 | v_y | m_0 \rangle = \frac{-i}{\hbar} \langle n_0 | \frac{\partial}{\partial k_y} | m_0 \rangle (E_{n_0} - E_{m_0}) =$$

$$= -\frac{i}{\hbar} \left\langle \frac{dn_0}{dk_y} \middle| m_0 \right\rangle \cdot (E_{n_0} - E_{m_0})$$

for all $m_0 \neq n_0$. Insert into v_y

$$v_y = \underbrace{\langle n_0 | v_y | n_0 \rangle}_{0} + \frac{ieE_x}{\hbar} \sum_{m_0 \neq n_0} \left\langle \frac{\partial n_0}{\partial k_y} \middle| m_0 \right\rangle \cdot \left\langle m_0 \middle| \frac{\partial n_0}{\partial k_x} \right\rangle + h.c.$$

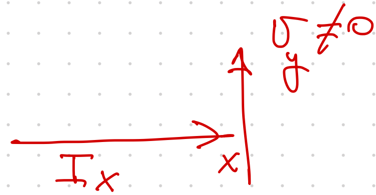
$\neq$

$$\sum_{m_0 \neq n_0} |m_0\rangle\langle m_0| = 1$$

from $\langle n_0 | v_y | n_0 \rangle = \frac{i}{\hbar} \langle n_0 | \frac{\partial}{\partial k} | n_0 \rangle (\underbrace{E_{n_0} - E_{n_0}}_{=0}) = 0$!

So finaly

$$v_y = \frac{ieE_x}{\hbar}\left(\left\langle \frac{\partial n_0}{\partial k_y}\middle|\frac{\partial n_0}{\partial k_x}\right\rangle - \underbrace{\left\langle \frac{\partial n_0}{\partial k_x}\middle|\frac{\partial n_0}{\partial k_y}\right\rangle}_{h.c.}\right) \neq 0$$



and since the plane wave part in $\boxed{|n_0\rangle = u_{nk}(\bar{x})\, \underbrace{e^{i\bar{k}\bar{x}}}_{\text{doesn't contribute}}}$ if no external is applied

we finaly get:

$$\boxed{v_y = \frac{ieE_x}{\hbar}\left(\left\langle \frac{\partial u_{nk}(\bar{x})}{\partial k_y}\middle|\frac{\partial u_{nk}(\bar{x})}{\partial k_x}\right\rangle - \left\langle \frac{\partial u_{nk}(\bar{x})}{\partial k_x}\middle|\frac{\partial u_{nk}(\bar{x})}{\partial k_y}\right\rangle\right)}$$

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 $u_{nk}(\bar{x})$.

$\Rightarrow$ 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 ($B=0$)

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

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

$T(R_n)$ commutes with $V(\bar{x})$ $\Rightarrow$ $T\,V(\bar{x}) = V(\bar{x} + \bar{R}_n) = V(\bar{x})$

it also commutes with ∇^n $n = 1, 2, \ldots$

$\Rightarrow$ it commutes with $\boxed{H = -\frac{\hbar^2}{2m}\nabla^2 + eV(\bar{x})}$ $B=0$

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

Now we apply an external mag. field B

$$\hat{H}_B = \frac{1}{2m}\left(i\hbar\nabla + e\hat{A}(x)\right)^2 + e\hat{V}(x)$$

where $\hat{A}(x) = -\frac{1}{2}(\hat{\bar{x}} \times \hat{\bar{B}})$

↑ in symmetric gauge

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

new $$\boxed{T_B(\bar{R}_n)} = e^{\bar{R}_n \cdot \left(\nabla - \frac{e}{i\hbar}\hat{A}(\bar{x})\right)}$$

$\underbrace{e}_{\text{no field}}$

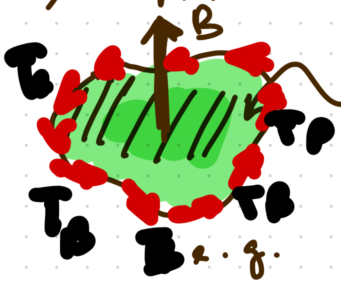
will commute with $i\hbar\nabla + eA(\bar{x}) \leftarrow$ Show THIS!

But now the problem is:

$$T_B(R_n)\,V(\bar{x}) = \underbrace{e^{R_n \cdot \frac{e}{i2\hbar}(\vec{x} \times \hat{\bar{B}})}}_{\text{extra phase}} \cdot V(x + R_n)$$

$= A(x)$

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



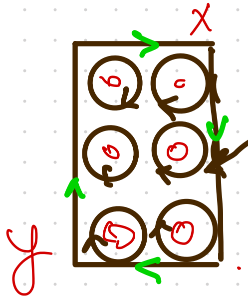
area size $\tilde{A}$

$$i\frac{eB}{\hbar}\cdot\tilde{A} = i\frac{2\pi eBA}{\hbar}$$

= if integer

e.g. Like in the Aharonov-Bohm

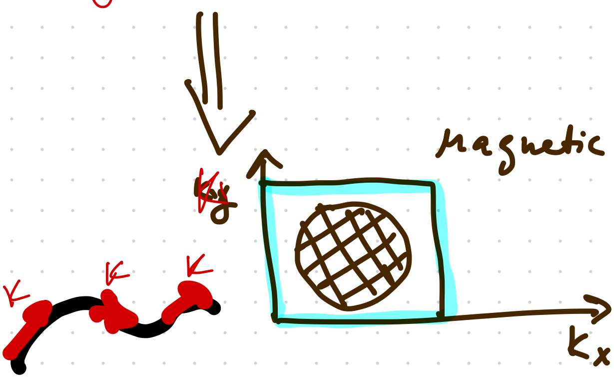
$$\oint A(\bar{x})d\bar{x} = \oiint \nabla \times A(\bar{x})\, d\tilde{A} = \oiint B\, d\tilde{A} = |\bar{B}| \cdot \tilde{A} \cdot \mathrm{sgn}(\bar{B} \cdot \tilde{A})$$



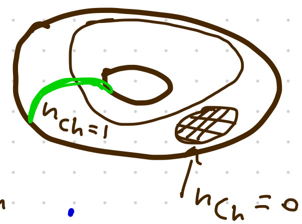
a magnetic unit cell

$p = 3$ pairs

magnetic BZ



$\Rightarrow$ Periodic boundary Condition



$j = -e \cdot v_y$

Finally we calculate

current $$j_y = -e \oiint_{\text{Mag. BZ}} \frac{1}{(2\pi)^2} \hat{v}_y(\bar{k})\, d\bar{k} =$$

$$= -e \oiint \frac{1}{(2\pi)^2} \frac{i e E_x}{\hbar = h/2\pi} \left(\left\langle \frac{\partial u_{n,k}(x)}{\partial k_y} \middle| \frac{\partial u_{n,k}(\bar{x})}{\partial k_x} \right\rangle - \left\langle \frac{\partial u_{n,k}(\bar{x})}{\partial k_x} \middle| \frac{\partial u_{n,k}(\bar{x})}{\partial k_y} \right\rangle \right) d^2\bar{k} =$$

density of states in k-space

$$j_y = \boxed{\frac{e^2}{h}} E_x \oiint_{MBZ} \frac{1}{2\pi i} \underbrace{\left(\langle \; \rangle - \langle \; \rangle \right)}\, d^2\bar{k}$$ ← Berry Curvature!

$\sigma_{xy} = \frac{e^2}{h} \cdot C_1 \cdot n$ ← size of BZ ↑ with B↑

But according to the experimental result the integral must be integer at the plateaux of the transverse $\sigma_{xy} = j_y/E_x = n e^2/h$ or $\sigma_{xy} = C_1 \cdot e^2/h$

often also labeled as C_1

This integer n_{ch} is called the Chern number

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

$$\langle \; | \; \rangle - \langle \; | \; \rangle =$$

$$= \left[\nabla_k \times \langle U_{n\bar{k}}(\bar{x}) | \nabla_k | U_{n\bar{k}}(\bar{x}) \rangle \right|_z :=$$

$$= \left[\nabla_k \times \underbrace{A_{Berry,n}(\bar{k})} \right]_z$$

where $\nabla_k = \frac{\partial}{\partial \bar{k}}$, and z is the 3^d component.

Recall the vector:

$$\bar{A}_{Berry,n}(\bar{k}) \equiv \langle U_{n,k}(\bar{x}) | \nabla_k | U_{n,k}(\bar{x}) \rangle$$

is the Berry connection

By the Stokes theorem if the integrand is continious

$$\sigma_{xy} = \frac{j_y}{E_x} = \boxed{\frac{e^2}{h} \cdot \frac{1}{2\pi i} \oint \bar{A}_{Berry,n}(k) \cdot d\bar{k}}$$

contour around MBZ

$$\boxed{:= \frac{e^2}{h} \cdot \frac{1}{2\pi i} \cdot \varphi_{Berry,n}} \leftarrow \text{Berry PHASE}$$

Reminder: Lets go back where we started: our quest for topology in QM

P(i)

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

Lets confirm the Q_I is the quantity we want:

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

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

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

$$= [\varphi(1) - \varphi(0)]/2\pi$$

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!

notice if the phase difference $\varphi(1) - \varphi(0) = 2\pi\cdot n$ ← integer

$\Rightarrow$ Q_I is integer!

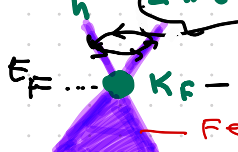
Let's compare this to σ_{xy}: $\mathbb{C}_1$ ← 1^{st} Chern number

$$\sigma_{xy} = \frac{j_y}{E_x} = \frac{e^2}{h}\cdot\overbrace{\frac{1}{2\pi i}\oint A_{Berry,n}(\bar{k})\,d\bar{k}}^{\mathbb{C}_1}$$

magnetic B_z

$$= \frac{e^2}{h}\underbrace{\frac{1}{2\pi i}\cdot\varphi_{Berry,n}}_{=\mathbb{C}_1 = Q_I(z)} =$$

a number of turns around a singularity in k-space in units of e^2/h



Fermi surface relat. e^- in solids

CHERN NUMBERS

Crystal electrons in Uniform electric field

from the previous section we described the velocity of a Bloch electron along y as

$$\langle v_k^n \rangle_y = \frac{1}{\hbar} \nabla_k \epsilon_k^{(n)} - \frac{e}{\hbar} E_x \Omega_{xy}^{(n)} \hat{y}$$

and demonstrated that

$$\sigma_{xy} = \frac{e^2}{h} \mathcal{C}_1^{(n)} \quad \text{where}$$

$$\mathcal{C}_1^{(n)} = \frac{1}{2\pi} \int_{MBZ} \Omega_{xy}^{(n)}(k)\, dk_x dk_y$$

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 BZ is an integer × 2π, which makes the invariant for w.f.

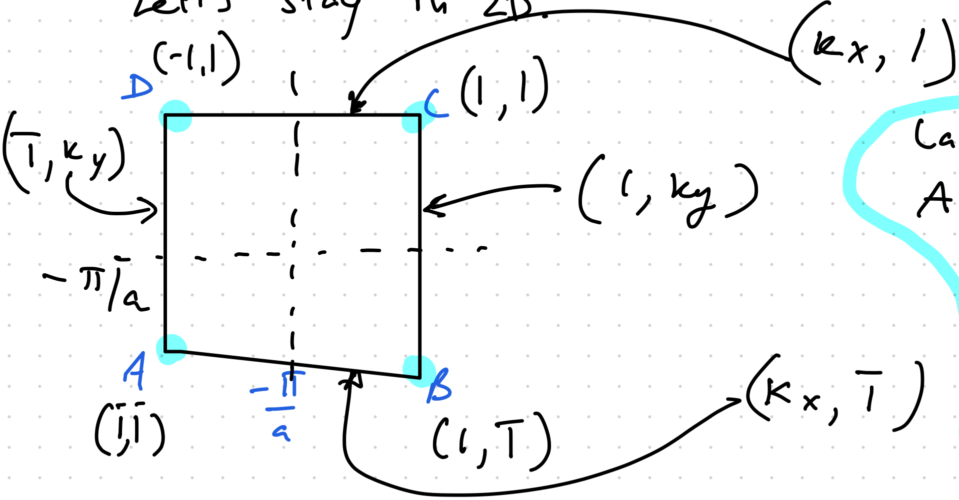
- Why do we need to know about the Chern number?

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

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

Here is another argument why the 1^{st} Chern nuber is integer.

Let's stay in 2D:



Labels are
$A = (-\frac{\pi}{a}\ -\frac{\pi}{a}) \equiv (\bar{1}, \bar{1})$
k_x and k_y are units of π/a

We can perform the Chern number calculation as a line integral along the boundary of the BZ.

$AB \to BC \to CD \to DA$

$$\left\{ \begin{array}{l} 1 \text{ is } k_x = k_y = \pi/a \\ \bar{1} \text{ is } k_y = k_y = -\pi/a \end{array} \right\}$$

$$2\pi C_1 = \oint_{ABCD} \bar{A}^{(n)}(k_x, k_y) \cdot d\bar{k} =$$

$$= \int_{AB} A_x^{(n)}(k_x, \bar{1})\, dk_x + \int_{BC} A_y(1, k_y)\, dk_y$$

$$+ \int_{CD} A_x^{(n)}(k_x, 1)\, dk_x + \int_{DA} A_y(\bar{1}, k_y)\, dk_y =$$

$$= \int_{\bar{1}}^{1} [A_x(k_x, \bar{1}) - A_x(k_x, 1)\, dk_y] +$$

$$+ \int_{\bar{1}}^{1} [A_y(1, k_y) - A_y(\bar{1}, k_y)]\, dk_y$$

if you recall $A_j^{(n)}(k_x, k_y) = i\langle U_k^{(n)} | \partial_{k_j} | U_k^{(n)} \rangle$ 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

$$|u^{(n)}_{k_x,1}\rangle = e^{i\varphi_x(k_x)}\,|u^{(n)}_{k_x,\bar{1}}\rangle$$

$$|u^{(n)}_{1,k_y}\rangle = e^{-i\varphi_y(k_y)}\,|u^{(n)}_{\bar{1},k_y}\rangle$$

Substituting these expressions into the integral we get

$$2\pi C^{(n)}_1 = \varphi_x(1) - \varphi_x(\bar{1}) - \varphi_y(1) +$$
$$+ \varphi_y(\bar{1})$$

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

$$|u^{(n)}_{k_A}\rangle \to |u^{(n)}_{k_B}\rangle \to |u^{(n)}_{k_C}\rangle \to |u^{(n)}_{k_D}\rangle$$
$$\to |u^{(n)}_{k_A}\rangle$$

by employing the phase difference between these states

$$|u^{(n)}_{\bar{1}\,\bar{1}}\rangle = e^{i\varphi_y(\bar{1})}\,|u^{(n)}_{1,\bar{1}}\rangle =$$
$$= e^{i(\varphi_y(\bar{1}) + \varphi_x(1)]}\,|u^{(n)}_{1,1}\rangle =$$
$$= e^{i[\varphi_y(\bar{1}) + \varphi_x(1) - \varphi_x(1) - \varphi_y(1)]}\,|u^{(n)}_{\bar{1},1}\rangle =$$

$$= e^{i[\varphi_y(\bar{1}) + \varphi_x(1) - \varphi_y(1) - \varphi_x(\bar{1})]} \cdot |u^{(n)}_{\bar{1}\bar{1}}\rangle$$

and b/c we end up with the same wave function which is single valued we must have

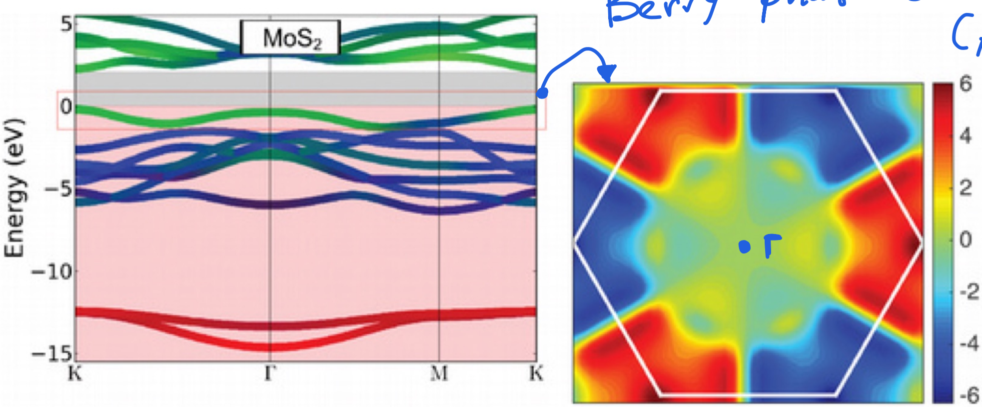
$$e^{i[\varphi_y(\bar{1}) + \varphi_x(1) - \varphi_y(1) - \varphi_x(\bar{1})]}$$

$$= 1 \Rightarrow \varphi_y(\bar{1}) + \varphi_x(1) - \varphi_y(1) - \varphi_x(\bar{1})$$

$$= 2\pi l \quad l - \text{integer}$$

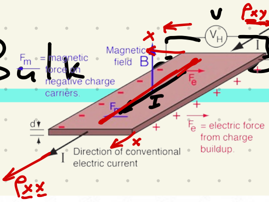
this proves that $\mathbb{C}_1$ must be integer.

Berry phase curvature ($\AA^{-2}$)



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 ($\AA^{-2}$) 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)].

QUANTUM ~~Surface~~ Bulk ~~spin~~ HALL EFFECT

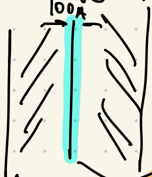


EXPERIMENTAL.

GaAs:Al

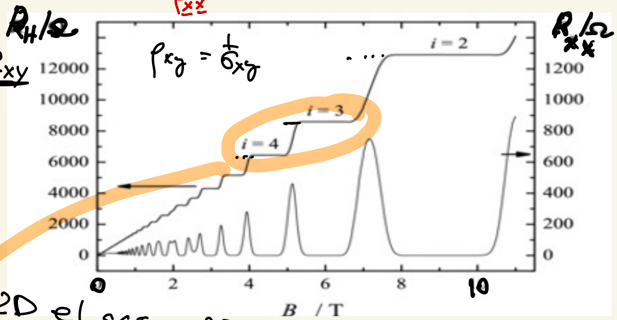
100Å

e

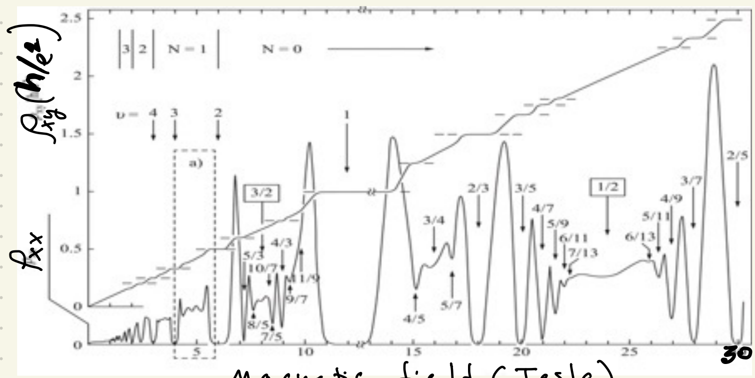


GaAs

2D el. gas = 2DEG



Integer Quantum Hall effect = IQHE



Fractional quantum Hall effect = FQHE

why we see this.

vacuum $C = 0$

surface

bulk $C = 1$

or

$g = 0 \quad \chi = 2 - 2g = 2$

surface

$g = 1 \quad \chi = 0$

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 $\bar{k}$ is governed by symmetry.

The dimension of a irreducable repres. at given $\bar{k}$ is equal to generacy at that point.

But in topo metals band degeneracy arizes from topology and close a gap at $\bar{k}$ not b/c. of symmetry

The condition for that was investigated by Herris in 1937!

Q: Starting with 2 band can we bring those bands into degeneracy by tuning Hamiltonian parameters:

e.g. for a system represented by

$$\boxed{H(k) = h_0(k)\sigma_0 + \bar{h}(k)\cdot\bar{\sigma}}$$

the details of coupling described by

$$\bar{h}(\bar{k}) = (h_1(\bar{k}), h_2(\bar{k}), h_3(\bar{k}))$$

of a <u>periodic function</u> of $\bar{k}$.

All the info about the topology of the w.f. is encoded in 4-real and periodic functions $(h_0(\bar{k}) \ldots h_3(\bar{k}))$ all defined on the whole BZ torus $\mathbb{T}^2$. The function $h_0(\bar{k})$ simply shifts the eigenvalues without affecting the eigenstates $\Rightarrow$ no effect on topo properties, but it important as it enters the dispersion

The eigenstates are (2×2 hamiltonian)

$$\varepsilon_{\pm}(k) = h_0(\bar{k}) \pm \sqrt{h_1^2(k) + h_2^2(k) + h_3^2(k)}$$

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

$h_j(k) \neq 0$ for each j, but

$\varepsilon_+(k) = \varepsilon_-(k)$ only if $h_j(\bar{k})$ for each $j > 0$ 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 $h_j(\bar{k})$ $j > 0$.

Here is the construction:

- each of the 3 equations $h_j(\bar{k}) = 0$ 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 $k_0 + \delta\bar{k}$ is then

$$H(\delta\bar{k}) = \epsilon_{k_0} + \hbar \nabla_k h_0(\bar{k})\, \sigma_0 + \sum_{j=1}^{3} \hbar \underbrace{\nabla_k h_j(k)\Big|_{\delta k=0}}_{=\bar{v}_\mu} \cdot \delta\bar{k} \cdot \sigma_j$$

if $\nabla_k h_0(k)\Big|_{\delta k=0}$ is $=0$ and the 3 velocity vectors $\bar{v}_\mu = \nabla_k h_\mu(\bar{k})\Big|_{\delta k}$ are orthogonal $\Rightarrow \mathcal{H}(k)$ will have the form of the anisotropic Weyl hamiltonian.

In 2D there only k_x k_y that we will vary $\Rightarrow$ no way to find simultaneous zeroes of 3 functions $h_j(k)$ without additional fine-tuning

$\Rightarrow$ in 2D without additional symmetry that constrains the number of idependent $h_j(\bar{k}) = 0$ the 2-bands avoid each other

- without constraint we can only get <u>accidental</u> two-fold degeneracy of bands in 3D - solids.

- The dispersion $\epsilon(k)$ is linear and similar to Weyl eqn.

Most important, if $h_0(k) = 0$ or $|\vec{d}| = 0$ the $\mathcal{H}(k)$ is a 2-level system (spin) we used in the HW3?

We then can presume that the node at k_0 is the Berry curvature of

$$\Omega = \pm \frac{\Delta \hat{k}}{2|k|^2} \quad \text{where } \bar{\Delta k} = \bar{k} - \bar{k_0}$$

The B. curvature field is that of a magnetic monopole with '+' '—' charge.

- Consider only one node or '+' charge

$$\mathcal{H}(k) = \pm\, v\, \bar{\sigma} \cdot (\bar{k} - \bar{k_0})$$

- UNDER TRS

$k \to -k \qquad \sigma \to -\sigma \qquad \mathcal{H} \to \mathcal{H}' = \pm\, v \cdot \sigma(k + k_0)$

$\Rightarrow$ must be other node with $k = -k_0$ with the same charge

Under space inversion

$\bar{k} \to -\bar{k}$ and $\sigma \to \sigma \Rightarrow$

$$\mathcal{H} \Rightarrow \mathcal{H}' = \mp\, v\, \bar{\sigma}\cdot(\bar{k}+\bar{k}_0)$$

- IS requires there must be another node with $-\bar{k}_0$ with "$-$" charge.
- if <u>Both</u> TRS and IS present each node will two monopoles of opposite charges $= 0$

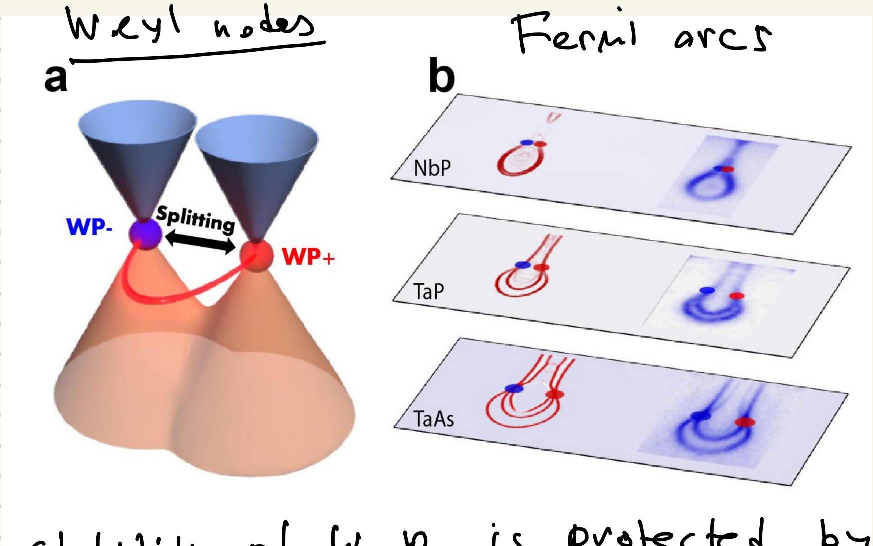
<u>Summery</u>

[In the absence of TRS <u>or</u> SI massless lattice fermions are required to come in <u>pairs</u> with opposite helicities, or Berry charges.]

NIELSEN – NIMOMIYA 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 W.p. is protected by the Gauss law: a Gaussian surface surrounding W.p detects its charge. It can oly dissapper if there is another oposslte monopole through the surface.

To realize the Weyl semimetal we need

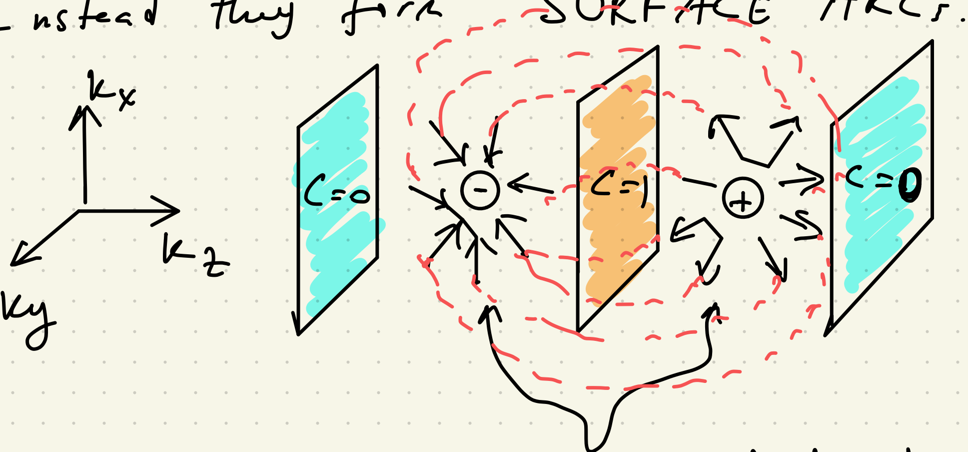
1) 3D crystal with non-degenerate bands by breaking either TRS or SI.
2) Points must be near Fermi surface where $h_0 = 0$ and v_j are orthogonal
   $h_0(k) \hat{=} 0$

Fermi ARCs

The Q.: now according to the bulk-surface correspondance, do W.S.s have the topo-surface states?

A:

Instead they form SURFACE ARCs.



a pair of Weyl points at $k_z = k_\pm$

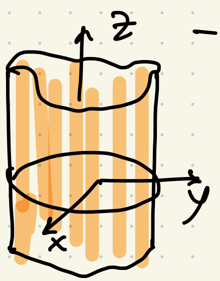
Note:
if we treat k_z as a parameter then for each value of k_z there is a band structure which depends on k_x and k_y.
But if $k_z \neq \pm k$ there is a gap in the band structure at F.S.

So we can define a Chern number for the system $\mathbb{C}(k_z)$.

Since $\mathbb{C}(k_z)$ is topological index it can change if the 2D band crossing $k = k_\pm$. So

$$C(k_- < k_z < k_+) \neq \mathbb{C} \text{ outside of } [k_- \; k_+]$$

- Consider the case of $\mathbb{C} = 1$ for $k_- < k_z < k_+$ and $C = 0$ otherwize

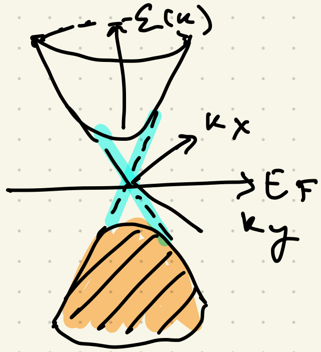
- 

— translationally invaricant in z

← finete in x, y

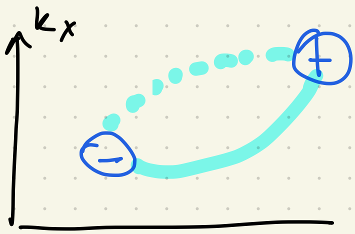
So k_z is a good quantum number

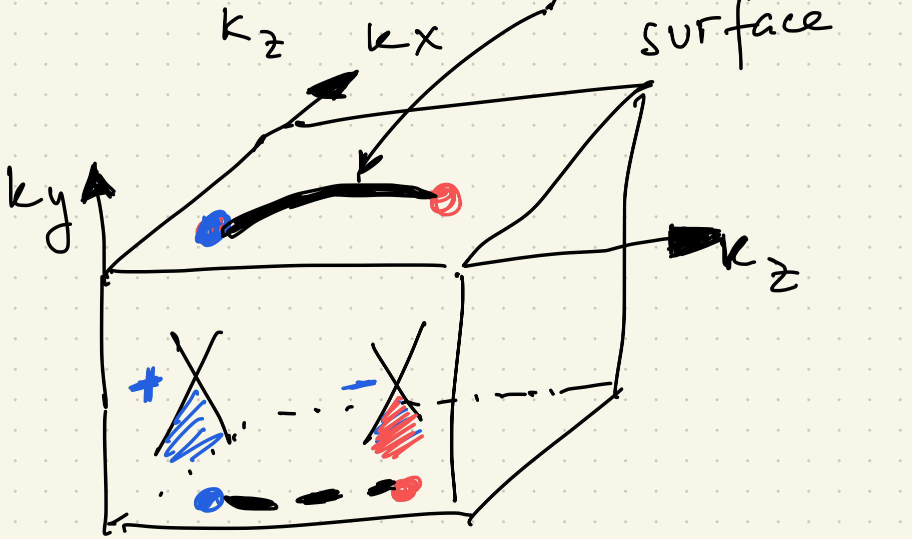
$\Rightarrow$ From the bulk - surface correspondence $\Rightarrow$ we will have the <u>edge</u> states for $k_- < k_z < k_+$ that intersect the Fermi surface.



for $k_+ < k_z < k_-$

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

Feynman's Epilogue

My last words I would say to you as your professor. Good luck!!!

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.