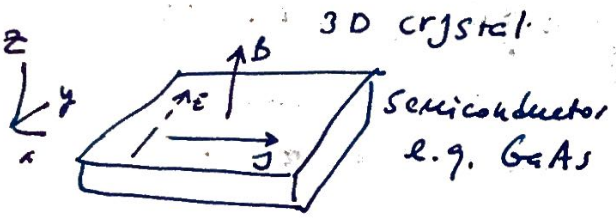
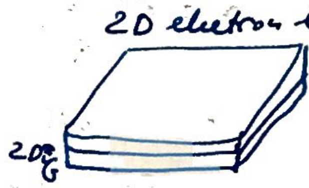
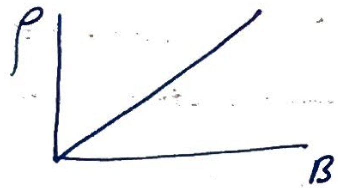
# Topology in solid State Physics

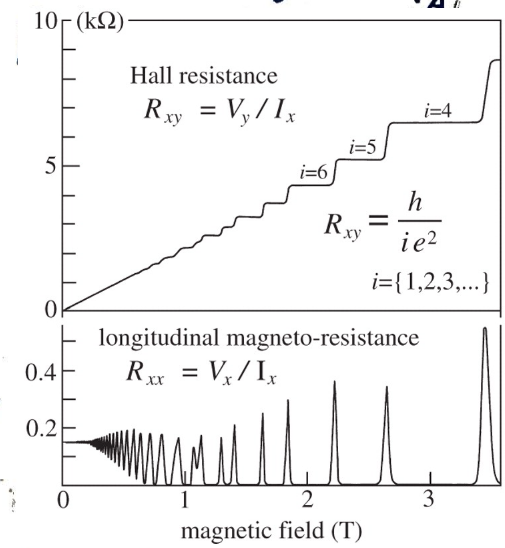
## Quantum Hall effect and Topological insulators

Here is a very interesting observation.




$\rho_{xx} = E_x / j_x$

$\rho_{xy} = E_y / j_x$

Based on the cylindrical symmetry

$$\rho_{xx} = \rho_{yy} \qquad \rho_{xy} = \rho_{yx}$$

From classical mechanics (Debye theory) $\rho_{xy} \sim B$

$e E_y = e v B \qquad j = e v n \Rightarrow \rho_{xy} = \frac{E_y}{J_x} = \frac{B}{en}$

Very useful but nothing too spectacular:

Quantum Hall effect and its connection to quantum electrodynamics

At low T and very very clean samples the 2DEG don't follow $\rho_{xy} \sim B$!

Instead is shows a series of very strange platoes. On the platoe $\sigma_{xy} = \frac{1}{\rho_{xy}}$ is quanties $= \frac{e^2}{h} n$ $\quad n = 1, 2, 3, \ldots$ and $\rho_{xx} = 0$!

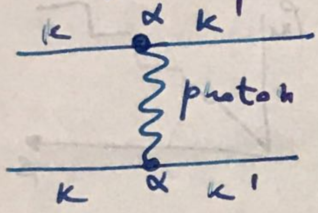
the filling factor.

Those platos are known as the Q. H. E.

Interestingly the value of conductivity can be expressed in terms of the fine structure constant:

$$\alpha = \frac{e^2}{\hbar c} \qquad \sigma_{xy} = n\frac{e^2}{\hbar} \Rightarrow = n \cdot \alpha \cdot c$$

The f.s. constant $\alpha$ measures the strength of quantum electrodynamics:




now $e^2 \sim$ coulomb potential
denominator $\sim c$

$$\alpha \sim \frac{\text{potential energy}}{\text{kinetic energy}}$$

If in our universe $\alpha = 0$ then electrons will not interact and in fact there will be <u>no photons</u> (no light - just imagine this).

If $\alpha$ is large the universe will be made of very <u>strongly entangled matter</u> which will make the presence of life impossible as we know it.

However $\alpha \sim \frac{1}{137}$ which is just 1% of the kinetic energy and we leave in the world with interactions $\equiv$ photons $\equiv$ light and yet we can do the perturbation theory.

Consider just kinetic energy as the unperturbed term, then in the 1st approx

$O(\alpha) \sim 1\%$, $O^2(\alpha^4) \sim 10^{-8}$!

Amazing but a condensed matter experiment can be as accurate as high energy physics in defining $\alpha$!

QED:

$$\alpha = \frac{e^2}{\hbar c} \sim \frac{1}{137}$$

CMP: $\alpha_{cmp} = \frac{e^2}{\hbar v_{Fermi}}$ for a typical solid $v_F \sim \frac{1}{100} - \frac{1}{1000} c$

So $\alpha_{cmp} = \frac{e^2}{\hbar v_F} \sim 1 \div 10$

so the perturbation theory don't work.

## QHE and Topology.

Before we answer why $\sigma_{xy}$ is quantized
Lets try to think why $\sigma_{xx} = 0$.

Q: if $\rho_{xx} = 0$ is it a superconductor / or "perfect metal

A: NOOooo.. The material is
~~SC~~ – ~~Conductor~~ – Insulator!
wow....

The material has 0 conductivity.

$$j = \sigma E \,, \qquad E = \rho j \qquad \rho = \frac{1}{\sigma}$$

This is only true if $j$ and $E$ are in the same direction. However more generally:

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \cdots & \sigma_{xz} \\ \vdots & \ddots & \vdots \\ \sigma_{zx} & \cdots & \sigma_{zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

if all but $\sigma_{xx}\, \sigma_{yy}\, \sigma_{zz}$ are not zero

$j = \sigma E$ and $\rho = \frac{1}{\sigma}$ but for 2D

$$\begin{pmatrix} j_x \\ j_y \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \end{pmatrix}$$ and the resistivity "

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix} \begin{pmatrix} j_x \\ j_y \end{pmatrix} \Rightarrow$$

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix}^{-1} =$$

$$= \frac{1}{\rho_{xx}\rho_{yy} - \rho_{xy}\rho_{yx}} \begin{pmatrix} \rho_{yy} & -\rho_{xy} \\ -\rho_{yx} & \rho_{xx} \end{pmatrix}$$

Now lets go to to the platoe where $\rho_{xx} = \rho_{yy} = 0$

$$\begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix} = \begin{pmatrix} 0 & \rho_{xy} \\ \rho_{yx} & 0 \end{pmatrix} \Rightarrow \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} = -\frac{1}{\rho_{xy}\rho_{yx}} \begin{pmatrix} 0 & -\rho_{xy} \\ -\rho_{yx} & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 1/\rho_{yx} \\ 1/\rho_{xy} & 0 \end{pmatrix} \Rightarrow \sigma_{xx} = \sigma_{yy} = 0$$ NO CONDUCTIVI[TY]

so the system is INSULATOR.

But between the plateaus the conductivity is non zero and as such it's METAL.

$\rho_{xx} \neq 0$ and $\sigma_{xx}$ and $\sigma_{yy} \neq 0$.

## SUMMARY OF EXP. FACTS ABOUT QHE.

1. When we vary the external field

- we can turn system ... ins $\leftrightarrow$ metal $\leftrightarrow$ ins. $\leftrightarrow$ metal ...
- each insulating state corresponds to a plateau of $\rho_{xy}$ and the step between 2 neighboring plateaus is metallic.
- transport for the metalic states is NOT universal, and changes from sample to sample.
- The insulating state is UNIVERSAL. $\rho_{xx}=0$ and $\sigma_{xx}=0$ and $\sigma_{xy}$ is quantized.

WHY IQH state is insulator?

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LANDAU LEVELS.

Lets solve this problem quantum mechanically. In 2D for a charge neutral particle $q=0$. the Schrödinger equ:

$$i\frac{\partial\psi(x,y)}{\partial t}=\left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2+\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y}\right)^2\right]\psi(x,y)$$

with $H=\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2+\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y}\right)^2$

Now lets include charge and its connection to E and B. He we will use a minimal coupling which tells that we change momentum $\vec{P}\rightarrow\vec{p}+\frac{e\vec{A}}{c}$ $A=$ vector potential

and $i\frac{\partial}{\partial t}\rightarrow i\frac{\partial}{\partial t}-\frac{e}{c}\phi$ $\phi=$ electric potential

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$$\left(i\frac{\partial}{\partial t} - \frac{e}{c}\Phi\right)\Psi(x,y) = \left[\frac{1}{2m}\left(-i\hbar - \frac{e}{c}A_x\right)^2 + \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y} - \frac{e}{c}A_y\right)^2\right]\Psi(x,y)$$

$$i\frac{\partial}{\partial t}\Psi(x,y) = \left\{\left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} - \frac{e}{c}A_x\right)^2 + \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y} - \frac{e}{c}A_y\right)^2\right] + \frac{e}{c}\Phi\right\}\Psi(x,y)$$

$$H = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} - \frac{e}{c}A_x\right)^2 + \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y} - \frac{e}{c}A_y\right)^2 + \frac{e}{c}\Phi$$

Since $E=0$ we can set $\Phi = 0 \Rightarrow$

$$\nabla\times A = \frac{\partial}{\partial x}A_y - \frac{\partial}{\partial y}A_x = B$$

from E & M we know that A is not observable i.e. for the fixed B field, A is not uniquely defined. $\nabla\times A = B$ $A' = A + \nabla\chi$ is also the vector potential for the same field $\nabla\times A' = B$. We can choos any A as long as as $\nabla\times A = \nabla\times A'$. Now lets apply the magnetic field along z : $B_z$ Then we can use 2 options : $A_x = 0$ $A_y = Bx$ (the Landau gage)

$\left.\begin{array}{l}\frac{\partial}{\partial x}A_y = B \\ \frac{\partial}{\partial x}A_x = 0\end{array}\right\}$ $\nabla\times A = B$. $A_x = -\frac{By}{2}$ and $A_y = \frac{Bx}{2}$ (the symmetric gage)

## Energy spectrum

$$H = \left[\frac{\hbar^2}{2m}\left(-i\frac{\partial}{\partial x}\right)^2 + \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y} - \frac{e}{c}Bx\right)^2\right];$$

Static Sch. equation: $H\Psi = E\Psi$

in the Landau gage $[p_y, H] = 0$ therefore we can find common eigen states for $p_y$ and $H$.

$$\Psi(x,y) = f(x)\, e^{-ik_y y}$$

$$-\frac{\hbar^2}{2m} f''(x) + \frac{1}{2m}\left(\hbar k_y - \frac{e}{c}Bx\right)^2 f(x) = \epsilon f(x)$$

(for $p_y$ the eigenvalue $\hbar k_y$), lets rewrite it:

$$-\frac{\hbar^2}{2m} f''(x) + \frac{e^2}{2mc^2}B^2\left(x - \frac{c\hbar}{eB}k_y\right)^2 f(x) = \epsilon f(x)$$

$$-\frac{\hbar^2}{2m} f''(x) + \frac{K}{2}(x - x_0)^2 f(x) = \epsilon f(x)$$

where $x_0 = \frac{c\hbar}{eB}k_y$ $\quad K = \frac{e^2B^2}{mc^2}$; $x_0 = \ell_c^2 k_y$ where $\ell_c^2 = \frac{c\hbar}{eB}$

now this equation looks like the harmonic oscillator:

Recall from your QM class, the solution is

$$\begin{cases} \Psi_{n,k_y}(x,y) = \phi_n(x - x_0)\, e^{-ik_y y} & \text{with} \\ \epsilon_{n,k_y} = \left(n + \frac{1}{2}\right)\hbar\omega = \left(n + \frac{1}{2}\right)\hbar\sqrt{\frac{K}{m}} = \left(n + \frac{1}{2}\right)\underbrace{\frac{eB\hbar}{cm}}_{\omega_c} \end{cases}$$

$n = 0, 1, 2, 3 \ldots$

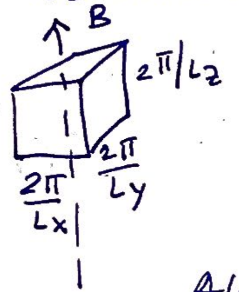
So the electrons are quantized in x-y and have continuous translation along z; so the total E

$$E = E(n, k_y) + \frac{\hbar^2}{2m}k_z^2 = \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2}{2m}k_z^2$$

If we include the spin of the electron then each level will split into 2 sublevels $\pm g_e \mu_B \sigma H$

Since the energy spectrum is dramatically affected we need to see what happens to the electronic density of states.

We start with




$\Rightarrow$ ? $\Rightarrow k_x$ and $k_y$ are quantized in units $\frac{2\pi}{L_x}$ and $\frac{2\pi}{L_y}$

Also recall $x_0 = \frac{c\hbar}{eB} k_y = \frac{2\pi \ell_c^2}{L_y}$

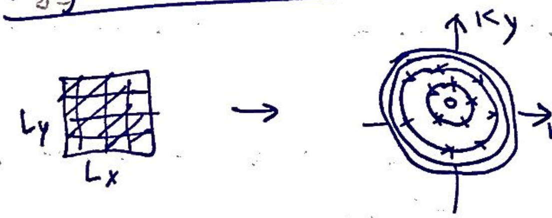
And the degeneracy of the level in 2D is:

$D = \frac{L_x}{\Delta x_0} = \frac{L_x L_y}{2\pi \ell_c^2}$ ; The total magnetic flux through the x-y plane is

$\Phi = H L_x L_y$ and the flux quantum: $\phi_0 = \frac{\hbar c}{e} \Rightarrow$

$D = \frac{\Phi}{\phi_0} \overset{or}{\Rightarrow}$ the number of states = number of the flux quanta in units of $\frac{\hbar c}{e}$!

The <u>PHYSICAL MEANING</u>:



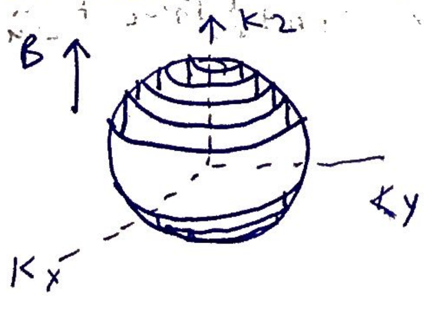

After applying the magnetic field points distributed in the $k_x - k_y$ area get spread out onto concentric circles with energies $\frac{\hbar\omega_c}{2}, \frac{3}{2}\hbar\omega_c, \frac{5}{2}\hbar\omega_c \dots$

But the total number of states remain the same. To show this lets calculate the number of states per unit area per unit energy and no spin

$$g(E) = \frac{1}{L_x L_y} \frac{D}{\hbar\omega_c} = \frac{m}{2\pi\hbar^2}$$

= which is the same as $= g^{2D}(E)$ without magnetic field attached.

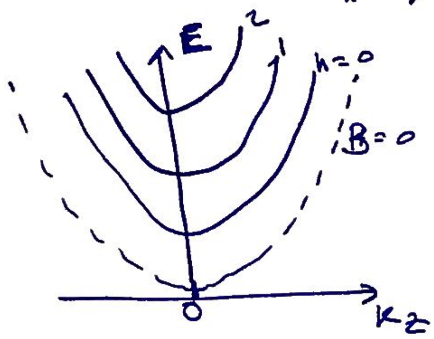
Now lets extend this to 3D:

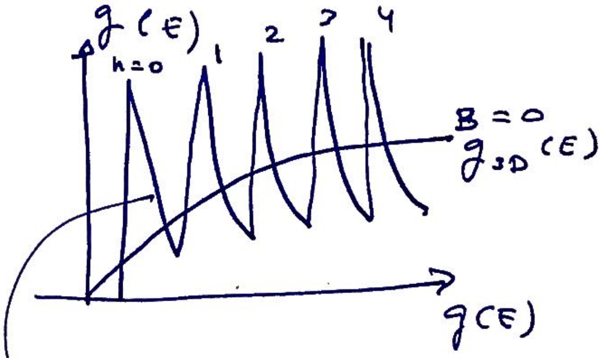



Note $k_z$ is still a good quantum number so we can plot $\epsilon(k_z)$ vs. $k_z$ as bands also known as the <u>Landau subbands</u>

Overall for 3D we have:

$$g_{3D}(E) = \frac{1}{(4\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \hbar\omega_c \sum_n \left[E - (n+\tfrac{1}{2})\hbar\omega_c\right]^{-1/2}$$

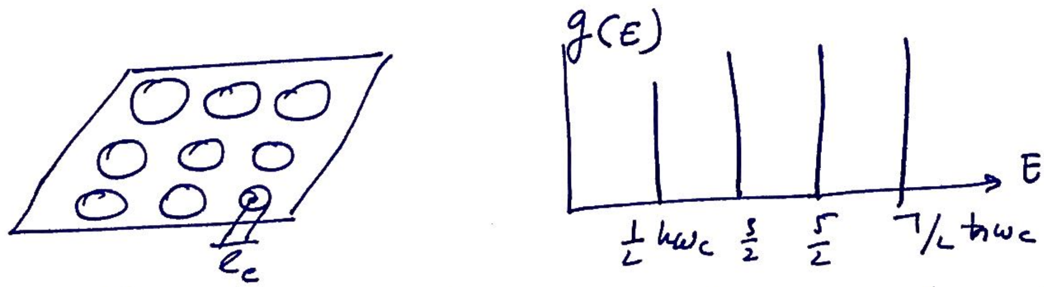



1D spikes from the states on the circumference of the circles.

$$g_{1D}(E) = \frac{1}{4\pi}\left(\frac{2m}{\hbar^2}\right)^{1/2}(E-E_n)^{-1/2}$$

For 2D this is very interesting



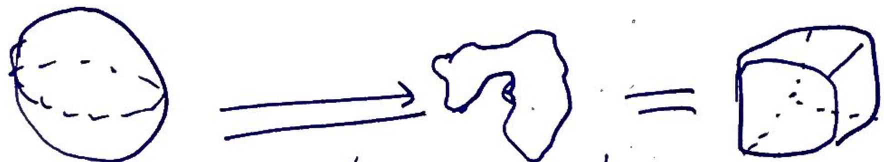

If we apply E along x-direction we going to have the famous QHE.

On the Landau levels: electrons colaple into a set of cylinder where they increase their degeneracy and move on the circles with $\omega_c$ frequency.
Moving electrons introduce flux through the cylynder with the flux # equal to the # of electrons in units of $\Phi_0 = \frac{\hbar c}{e}$

## Topology and insulators

Topology came from 3D real space but now moved to the Hilbert space

Def.: if a manyfold $M_1$ can be adiabatically transformed into $M_2$, their topology is the same.



To distinguish between them we introduce an object called index (a topo index)

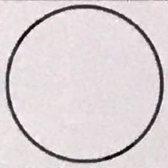
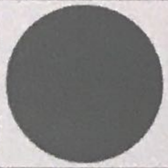
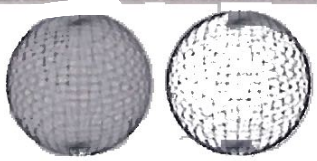
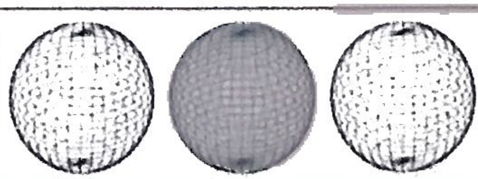
the same topo object = the same index

For 2D:

$$\chi_M = \frac{1}{2\pi} \oiint K\, dS$$ (the Euler characteristic)

| Name | Image | Vertices $V$ | Edges $E$ | Faces $F$ | Euler characteristic: $V-E+F$ |
|---|---|---|---|---|---|
| Tetrahedron | | 4 | 6 | 4 | 2 |
| Hexahedron or cube | | 8 | 12 | 6 | 2 |
| Octahedron | | 6 | 12 | 8 | 2 |
| Dodecahedron | | 20 | 30 | 12 | 2 |
| Icosahedron | | 12 | 30 | 20 | 2 |

See WIKIPEDIA on the EULER CHARACTERISTIC

| Name | Image | Euler characteristic |
|---|---|---|
| Interval |  | 1 |
| Circle |  | 0 |
| Disk |  | 1 |
| Sphere |  | 2 |
| Torus (Product of two circles) |  | 0 |
| Double torus |  | −2 |
| Triple torus |  | −4 |
| Real projective plane |  | 1 |
| Möbius strip |  | 0 |
| Klein bottle |  | 0 |
| Two spheres (not connected) (Disjoint union of two spheres) |  | 2 + 2 = 4 |
| Three spheres (not connected) (Disjoint union of three spheres) |  | 2 + 2 + 2 = 6 |

we locally fit the surface ~~for~~ to a particular circle and the $1/R$ is the local curvature $\kappa$

Among all the curvatures the largest and the smallest curvatures $\kappa_1 = \frac{1}{R_1}$ and $\kappa_2 = \frac{1}{R_2}$ are the principal curvatures. The gaussian curvature

$$K = \frac{1}{\kappa_1} \cdot \frac{1}{\kappa_2}$$

For sphere $\kappa = \frac{1}{R_1} = \frac{1}{R_2}$ $\qquad K = \frac{1}{R^2}$

For a saddle point $\kappa_1 > 0$ and $\kappa_2 < 0$

$\Rightarrow K = \kappa_1 \cdot \kappa_2 \leq 0$

Th: For any well-behaved 2D surface the $\oiint K \, dS = 2\pi \cdot n = \chi_M$ so it's quantized! Also for the surfaces with the same topology $\chi_M$ are the same.

Th: For any orientable closed surface $\chi_M$ is always an even integer.

Orientable means we can distinguish two sides of the surface. If we cannot then $\chi_M$ is ODD (e.g. a Möbius strip)

— $\chi_M$ is a topological index only when the surface has no boundaries. Otherwise, it's not quantazided and not Topological.

## Other topological properties:

① Topology and handles

$\chi_M$ is related to the genus of a surface (or manyfold)

$$\chi_M = 2(1-g).$$ where $g$ is the number of handles of the object.

e.g. Sphere $g=0$ torus $g=1$

a coffee mug = a donut. , or

3-handled cup = a pretzel = a triple torus

② $\chi_M$ and polyhedrons.

To define $\chi_M$ we can draw a grid of polyhedrons

$$\chi_M = \underset{\text{Corners}}{V} - \overset{\text{edges}}{E} + \underset{\text{faces}}{F}$$ e.g. since a sphere has $\chi_M = 2$ we know that $V-E+F=2$

③ Topology and hair vertex

If we draw a vector at each point of the surface. We get a vector field, which <u>may have vortices</u>. Now we define a <u>verticity</u> which is an integer number $n$, The total verticity $\chi_M = \sum n$.

ignore!

~~Quantum Hall effect of an insulator~~

~~We start with the equation $E_n = \hbar\omega(n+\frac{1}{2})$ $n=0,1,2,\ldots$~~

~~We get equally spaced levels which are massively degenerate.~~

~~The massive degeneracy can be seen in the wavefunction~~

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For sphere $\chi_M = 2 = \sum n = 2 \neq 0$
( south and north poles)

The conclusion is, we cannot comb hair on the sphere without making the singularities (verteces).

## Topological index for an insulator

The Berry curvature and the Chern number.

for an insulator we can use the Bloch waves to define a curvature in the 2D - k space. for Bloch waves

$\psi_{n,k}(\bar{r}) = U_{n,k}(\bar{r}) e^{i\bar{k}\bar{r}}$, we define the k-space curvature (Berry curvature) as

$$\mathcal{F}_n(k) = \iint_{\text{unit cell}} |\nabla_k U_{n,k}(\bar{r})|^* \times \nabla_k U_{n,k}(\bar{r})\, d\bar{r} =$$

gradient $\nabla_k$ defines the vector in the k-space

$$= \epsilon_{ij} \iint_{\text{U.C.}} \left|\frac{\partial}{\partial k} U_{n,k}(\bar{r})\right|^* \frac{\partial}{\partial_k} U_{n,k}(\bar{r})\, dr$$

$\epsilon_{ij}$ = Levi-Civita symbol $\quad \epsilon_{xx} = \epsilon_{yy} = 0$
$\epsilon_{xy} = -\epsilon_{yx} = 1$

FROM the MATH P.O.V. the BERRY CURVATURE AND THE GAUSSIAN CURVATURE ARE THE SAME

The total Berry curvature is the topological index!

The topological index is defined as

$$C_n = \frac{1}{2\pi} \oiint_{BZ} \mathcal{F}_n(k)\, d\bar{k} \equiv \text{the Chern number}$$

For each band $n$, we can define such a number $C_n$ and for an insulator the total Chern #:

$$C = \sum_n C_n$$

$n$ ← over the filled bands

- The total chern number $C$, is the same as the number of chiral edge states.
  e.g. if $C=0$ we have a trivial insulator without edge states $\sigma_{xx} = \sigma_{xy} = 0$.
- If $C \neq 0$ we call such an insulator a TI or the Chern insulator.
  This insulator will have the edge states with $\boxed{\sigma_{xx} = 0}$ and $\boxed{\sigma_{xy} \neq 0 = C \frac{e^2}{\hbar}}$ for the Hall conductivity.
- Let me also claim without a proof.
  For a metal ~~or~~ an insulator, the Hall conductivity is the total Berry phase curvature summed over all occupied states. For metal we sum up over occupied (valence) and partially occupied bands (conduction bands):

$$\sigma_{xy} = \frac{e^2}{\hbar} \sum_{n,\,\text{valence band}} \left[\frac{1}{2\pi}\int_{BZ} d\bar{k}\, \mathcal{F}_n(\bar{k})\right] + \frac{e^2}{\hbar} \sum_{n,\,\text{conduction}} [\ldots]$$

- Few important points. For the gaussian curvature, the total K is only quantized if the surface has no boundaries.

- For the Berry curvature is the same.
  if we integrate over the whole BZ we will have a quantized Chern number.
- However, if we integrate over a part of BZ the C is non integer.

- For a metal we need to integrate only over the filled states or the Fermi sea and as such there is a boundary set by the Fermi surface. As such $C_0$ is not quantized. That is why we have no quantized Hall conductivity for metals but we do have this for insulators.

- So by Chern # we define TI but not Topological metals.

OTHER TOPOLOGICAL INDICES.

If in addition to the C number, we demand a certain symmetry to be present e.g. time-reversal (TR) we can introduce different topo indeces.

If any of these indees are non-zero the insulator is also a TI.
This kind of insulators also called the symmetry-protected insulators (SPTI), with the common properties:

- One of the indees is non-zero.
- The bulk is an Insulator, but the edge is a metalic state
- The edge state is different from a simple metal in d-1 dimensions. (e.g. 1/2 of the ordinary metal)
- The edge states may have some quantization effect.
- If the symmetry is broken the edge state disappear.

Note: if we assume no symmetry the only TI is the Chern insulator, which is defined in the even space dimensions, i.e. we can have QHE only in 2D but not in 3D.

Note: for SPTIs they can exis for both 2D & 3D if we preserve TR symm. (e.g. NO MAGNETISM)
In 1D we need a very special symmetry called the chiral symmetry to get a TI.

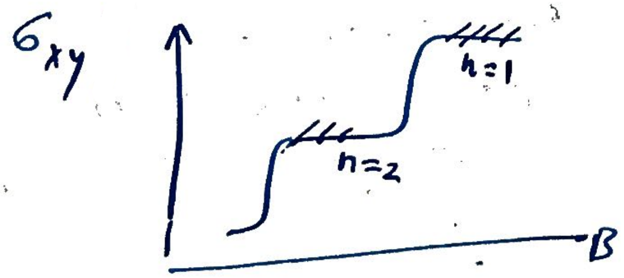
Q. Why TI have metalic states at the edge?

Consider


vacuum is an insulator (though trivial) with $C=0$ inside the TI $C\neq 0$.

NB! Topology never changes in a smooth way! We cannot deform a sphere into a torus similarly we cannot transform a trivial or a band insulator into a TI, thus the insulating states need to be destroyed by closing a band gap, or we get a metal.

Q. Why there is a metalic region between two plateaus?




different plateaus have different topological indeces $n$.
So the story as above to go from $n=1 \to n=2$ need to close a gap to destroy the topology. $\Rightarrow$ metal.

Q Why the Hall conductivity is so exact in a Chern TI?

19

Since the Hall conductivity is determined by topology of the wave function it's very robust and precise.

So as long as any perturbation is not changing topology (or destroy protective symmetry) $\sigma_{xy}$ will be the same for any sample.

In order to do this via some kind of perturbation we need to close a gap first (via doping for example) and only then we can change $\sigma_{xy}$.

So technically the error bar in $\sigma_{xy}$ is 0. (well within how well we know $\hbar$ and $e$)

Q. So far you talked about non-interacting $e^-$. What if you turn e-e interactions?

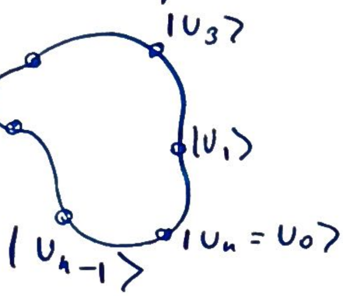
For weakly interacting electrons the same connection between topology and Hall (the Berry connection) still remains.
No proof here.

Based on lectures by D. Vanderbilt



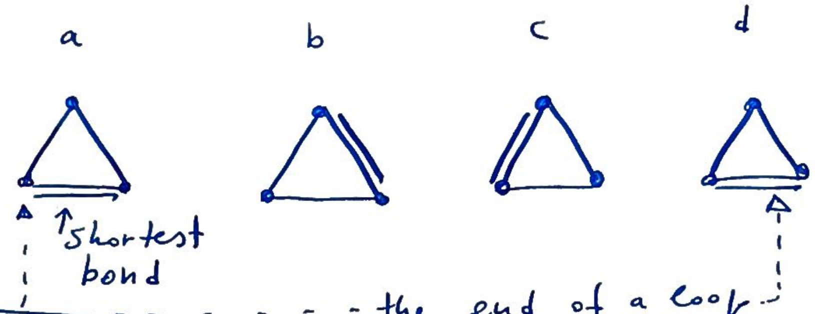
# More about Berry phase

BP describes phase accumulation due to a motion of some complex vector around a close loop in the complex vector space.




**DESCRETE VERSION**

For a specific example, let's consider a triatomic molecule.




The BP is defined as

$$\boxed{\phi = -\mathrm{Im}\ln\left[\langle u_0|u_1\rangle\langle u_1|u_2\rangle\dots\langle u_{N-1}|u_0\rangle\right]}$$

For a complex vector $z = |z|e^{i\phi}$ $\quad \mathrm{Im}\ln z = \phi$.

$U_B = R^{120°}|U_a\rangle \dots$

Consider now our triatomic molecule

$$|u_a\rangle = |u_d\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad |u_b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\e^{2\pi i/3}\end{pmatrix} \quad |u_c\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\e^{4/3\pi i}\end{pmatrix}$$

then BP is given by:

$$\phi = -\mathrm{Im}\ln\left[\langle u_a|u_b\rangle\langle u_b|u_c\rangle\langle u_c|u_d\rangle\right] =$$
$$= -\mathrm{Im}\ln\left[\left(\frac{e^{\pi i/3}}{2}\right)^3\right] = -\pi.$$

At least mathematically the BP is independent of individual phases of $|u_j\rangle$. Let's introduce a new set of N states

$$|\tilde{u}_j\rangle = e^{-i\beta_j}|u_j\rangle$$

$\beta_j$ is real

We can show that in this case the BP is unaffected as $e^{\pm i\beta_j}$ along the path will cancel out.

So we should say that <u>BP is gauge invariant</u> and as such perhaps describes some kind of physics.

~~THE CONCEPT OF A PARALLEL TRANSPORT~~

~~Suppose we have a chain of states $|U_0\rangle$ $|U_1\rangle$ ... $|U_N\rangle$ with no special phase relation. Let's define a new set, except of states $|\tilde{U}_0\rangle$ $|\tilde{U}_1\rangle$ ...~~

## Continuous formulation of BP

In this formulation we ~~para~~ parametrize the path by a real variable $\lambda$ such that $|u_\lambda\rangle$ traverses the path as $\lambda$ evolves from 0 to 1, i.e. $|u_{\lambda=0}\rangle = |u_{\lambda=0}\rangle$ and $|u_\lambda\rangle$ is a smooth function of $\lambda$. Lets try to derive an expression similar to the descrete version.

$$\ln \langle u_\lambda | u_{\lambda+d\lambda}\rangle = \ln \langle u_\lambda | \left( |u_\lambda\rangle + d\lambda \frac{d|u\rangle}{d\lambda} + \dots \right)$$

$$= \ln \left(1 + d\lambda \langle u_\lambda | d_\lambda u_\lambda\rangle + \dots\right) = d\lambda \langle u_\lambda | \partial_\lambda u_\lambda \rangle + \dots$$

$$\partial_\lambda \equiv \frac{d}{d\lambda}$$

Then BP is: $\boxed{\phi = -\mathrm{Im} \oint \langle u_\lambda | \partial_\lambda u_\lambda\rangle d\lambda}$

$$\mathrm{Re} \langle u_\lambda | \partial_\lambda u_\lambda\rangle = \langle u_\lambda | \partial_\lambda u_\lambda\rangle + \langle \partial_\lambda u_\lambda | u_\lambda\rangle = \partial_\lambda \langle u_\lambda | u_\lambda\rangle = 0$$

$\Downarrow$ $\langle u_\lambda | \partial_\lambda u_\lambda\rangle$ is pure imaginary and.

$$\boxed{\phi = \underbrace{\oint \langle u_\lambda | i\partial_\lambda u_\lambda\rangle d\lambda}}$$

Berry connection or Berry potential

$$A(\lambda) = \langle u_\lambda | i\partial_\lambda u_\lambda\rangle = -\mathrm{Im} \langle u_\lambda | \partial_\lambda u_\lambda\rangle$$

In terms of $A(\lambda)$:

$$\phi = \oint A(\lambda)\, d\lambda$$

Q: How Berry connection changes under gause transformation?

$$|\tilde{u}_\lambda\rangle = e^{-i\beta(\lambda)}|u_\lambda\rangle$$
$\uparrow$ real function

$$\tilde{A}(\lambda) = \langle\tilde{u}_\lambda|\partial_\lambda \tilde{u}_\lambda\rangle = \langle u_\lambda|\, e^{i\beta(\lambda)}\, i\partial_\lambda\, e^{-i\beta(\lambda)}|u_\lambda\rangle =$$
$$= \langle u_\lambda| i\partial_\lambda|u_\lambda\rangle + \underbrace{\beta'(\lambda)}_{\frac{\partial\beta}{\partial\lambda}}$$

So B Potential is not gauge invariant! and it changes as:

$$\tilde{A} = A + \frac{d\beta}{d\lambda}.$$ But what about B Phase?

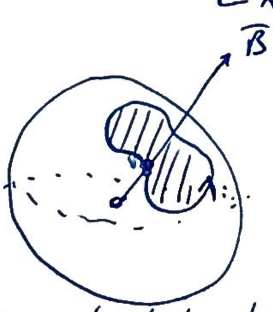
$$|\tilde{u}_{\lambda=1}\rangle = |\tilde{u}_{\lambda=0}\rangle \Rightarrow \beta_{\lambda=1} = \beta_{\lambda=0} + 2\pi m, \quad m = 0, 1 \ldots$$

$$\int_0^1 \frac{d\beta}{d\lambda}\, d\lambda = \beta_{\lambda=1} - \beta_{\lambda=0} = 2\pi m$$ so for

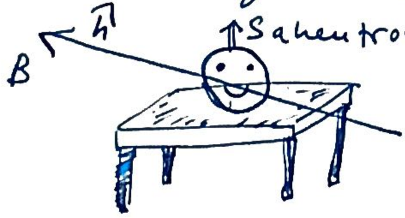
$$\tilde{\phi} = \oint \tilde{A}(\lambda)\, d\lambda = \underbrace{\oint \left(A + \frac{d\beta}{d\lambda}\right) d\lambda}_{=\phi} = \phi + 2\pi m$$

So BP is still gauge invariant!
You can think of BP as the phase which still left over after moving in the loop.

EXAMPLE




let me illustrate this by considering a real physical problem.
imagine we have an eigenvector which is a ground state of some $H_\lambda$. We can smoothly evolve the ground state by changing $\lambda$, which in our case can be magnetic B or electric fields E.




$\uparrow S$ a neutron at rest.

$$H = -\gamma B \cdot \underbrace{S}_{=\frac{\hbar}{2}\hat{\sigma}} = -\left(\frac{\gamma\hbar B}{2}\right)\hat{n}\cdot\hat{\sigma}$$

The ground state is independent of $|B|$ but depends on $\sigma$ operator.

So we can write instead $|U_n\rangle$ to emphasize that $|U\rangle$ depends on the direction of the magnetic field and not on its magnitude $|B|$.

Q: What's the BP of $|U_n\rangle$ as $\hat{n}$ carried around a loop in the magnetic field.

Lets try a simple descrete version:

① $\hat{n} \parallel \hat{z} \rightarrow$ rotate to $\hat{x} \rightarrow$ to $\hat{y} \rightarrow$ back to $\hat{z}$.

So we are tracing one octant of the sphere.

$$\phi = -\mathrm{Im}\ln\left[\langle\uparrow z|\uparrow x\rangle\langle\uparrow x|\uparrow y\rangle\langle\uparrow y|\uparrow z\rangle\right]$$

What we remember from QM 1 is that a spinor in arbitraty direction $\hat{n}$ is given by:


$$|\uparrow n\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \; e^{i\varphi} \end{pmatrix}$$

$$|\uparrow x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |\uparrow y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \qquad |\uparrow z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Ignoring the normalization factors:

$$\phi = -\mathrm{Im}\ln\left[(1)(1+i)(1)\right] = -\pi/4$$

$\boxed{\text{Exersize:}}$ Show that for N spinors taking N equally spaced values from 0 to $2\pi$ gives:

a) $$\phi = -N\tan^{-1}\left[\frac{\sin^2(\theta/2)\sin(2\pi/N)}{\cos^2(\theta/2) + \sin^2(\theta/2)\cos(2\pi/N)}\right]$$

b) find $\phi(\theta)$ for $N \to \infty$

c) for $\theta = 45°$ compute numerically $N = 3, 4, 6, 12 \ldots 100$ and compare to $N \to \infty$

THE END

# Topological Quantum Mechanics

Q. Why some insulators are interesting e.g. QHE and the other are trivial e.g. a piece of plastic?

Consider, QHE: ① $\sigma_{xy} \sim \hbar$. So quantum is important.
② Transport is a motion of charge. In QM charge is related to a conjugate variable of charge.
i.e. like $p$ is conjugate of $z$.
Invariant under $\phi \to \phi + \delta\phi$ implies the conservation of charge. So perhaps phase of the wave function is the key. Focus on phase. First, is phase of any importance?
A: relative yes, absolute no $\Rightarrow$ i.e:
$|\psi\rangle \to |\psi'\rangle = e^{i\varphi}|\psi\rangle \Rightarrow \langle\psi|A|\psi\rangle = \langle\psi'|A|\psi'\rangle$

However, $|\psi\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{1}{\sqrt{2}}|\psi_2\rangle \Rightarrow$

$$\langle\psi|P|\psi\rangle = \frac{\underbrace{\langle\psi_1|P|\psi_1\rangle}_{\bar{P}\ \text{in}\ \psi_1} + \underbrace{\langle\psi_2|P|\psi_2\rangle}_{\bar{P}\ \text{in}\ \psi_2}}{2} + \frac{\langle\psi_1|P|\psi_2\rangle + \text{conj}}{2}$$

The physical meaning of $\leftarrow$ is in the interference

$$|\psi'\rangle = \frac{1}{\sqrt{2}}|\psi_1\rangle + \frac{e^{i\varphi}}{\sqrt{2}}|\psi_2\rangle \Rightarrow$$

$$\langle\psi'|p|\psi'\rangle = \frac{\langle\psi_1|P|\psi_1\rangle + \langle\psi_2|P|\psi_2\rangle}{\sqrt{2}} + \frac{e^{i\varphi}\langle\psi_1|P|\psi_2\rangle + e^{-i\varphi}\langle\psi_2|P|\psi_1\rangle}{2} =$$

$$= \ldots + \cos\varphi \frac{\langle\psi_1|P|\psi_2\rangle + \langle\psi_2|P|\psi_1\rangle}{2}$$

↑ this can be measured!
AND VERY IMPORTANT

Common use of the phase is in condensed matter.
Phase of Bloch waves: Consider a particle moving in a periodic potential.

$$\left[-\frac{1}{2m}\nabla^2 + V(r)\right]\psi(r) = \epsilon\,\psi(r) \quad \text{where } V(\bar{r}) = V(\bar{r}+\bar{a})$$

The eigenfunctions of this equations:

$$\psi_{n,k} = U_{n,k}(r)\,e^{ikr} \leftarrow \text{Bloch wave functions}$$

Now what is the phase of the Bloch wave:
As usual in QM, doesn't matter, as it's invariant under global shift in the momentum space.

$\psi_{n,k}(r) = u_{n,k}(r)\, e^{ikr}$ $\psi'_{n,k}(r) = e^{i\varphi} u_{n,k}(r)\, e^{ikr}$
is the same.
What's interesting it is also invariant under local shift:

$\psi'_{n,k}(r) = e^{i\varphi(k)} u_{n,k}(r)\, e^{ikr}$. Which means that there is no mixing of waves with different $k$. as time goes on and on.

Let's focus on local phase symmetry:

Lets briefly review the concept of gauge in real space and then we will switch to the momentum space.

$$i\frac{\partial}{\partial t}\psi(r,t) = -\frac{\nabla^2}{2m}\psi(r,t) + V(r)\psi(r,t) \leftarrow \psi' \equiv e^{i\varphi}\psi(r)$$

$\psi'(r)$ will follow exactly the same equation as $\psi(r)$.
And we say the system is invariant under global phase shift. or global phase symmetry.

Remember, each symmetry implies the conservation of something.

e. g. $x \rightarrow x+a$ implies $-i\frac{\partial}{\partial x}$ conserved.
so here for $U(1)$ phase symmetry we expect
$-i\frac{\partial}{\partial \varphi}$ is conserved.

Now we switch to the Local $U(1)$ phase symmetry.
i.e $\varphi(r)$ $\psi(r,t) = e^{i\varphi(r,t)}\psi(r,t)$
is Sch. eq. still invariant? NO.

$\frac{\partial}{\partial t} e^{i\varphi} \neq e^{i\varphi}\frac{\partial}{\partial t}$ and $\nabla e^{i\varphi} \neq e^{i\varphi}\nabla$.
But can we make the equation invariant?
Yes if we introduce some "charge particle" trick.

Lets recall the problem of motion of a chaged particle $e$. We change its $\bar{p} \to \bar{p} + e\bar{A}/c$ and change $\frac{i\partial}{\partial t} \to \frac{i\partial}{\partial t} - e\bar{\Phi}$

$$\left(i\hbar \frac{\partial}{\partial t} - e\bar{\Phi}\right)\psi(r,t) = \left[\frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}A\right)^2\right]\psi(r,t) + V(r)\psi(r,t)$$

$$\left(i\hbar \frac{\partial}{\partial t} - e\bar{\Phi} + \hbar\frac{\partial \phi(r,t)}{\partial t}\right)\psi'(r,t) = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}A - \hbar\nabla\phi(r,t)\right)^2\psi(r,t) + V(r)\psi(r,t)$$ if we define

$$\bar{\Phi}' = \bar{\Phi} - \frac{\hbar}{e}\frac{\partial\varphi(r,t)}{\partial t} \quad \text{and} \quad A' = A + \frac{c\hbar}{e}\underset{\nabla}{\frac{\partial\phi(r,t)}{\partial r}}$$

we get: $\left(i\hbar\frac{\partial}{\partial t} - e\bar{\Phi}'\right)\psi'(r,t) = \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}A'\right)^2\psi(r,t) + V(r)\psi(r,t)$

The change of $\boxed{\begin{array}{l}\bar{\Phi}' \to \bar{\Phi} - \frac{\hbar}{c}\frac{\partial\varphi(r,t)}{\partial t} \\ A' \to A + \frac{c\hbar}{e}\frac{\partial\varphi}{\partial r}\end{array}}$ and

is called the gage thansformation, and it keeps physics $\bar{E}$ and $\bar{B}$ the same. More popular way to write it is to absorb $\frac{c\hbar}{e}$ into $\varphi$:

$$\boxed{\begin{array}{ll}\bar{\Phi} \to \bar{\Phi}' = \bar{\Phi} - \frac{1}{c}\frac{\partial\varphi}{\partial t} & A \to A' = A + \nabla\varphi(r,t) \\ & \psi(r,t) \to \psi' = \psi(r,t)\, e^{i\frac{e}{c\hbar}\varphi(r,t)}\end{array}}$$

The local phase invariance is related to the gage field.

## Berry connection and Berry curvature

Lets introtude the Berry connection

$$\bar{A}_n = -i\langle U_{n,k}|\nabla_k|U_{n,k}\rangle$$

As you can immidoatelly see this is a guage field in the momentum space, very similar to the vector potential.

$|U_{n,k}\rangle \to e^{i\varphi_n(k)}|U_{n,k}\rangle$ to make the Bloch f. to be local phase invariant we need to do this:

$$A_n \to A_n' = -i\langle U_{n,k}|e^{-i\varphi_n(k)}\nabla_k e^{i\varphi_n(k)}|U_{n,k}\rangle =$$

$$|U_{n,k}\rangle \to e^{i\varphi_n(k)}|U_{n,k}\rangle$$

$$A_n \to A_n' = -i\langle U_{nk}|e^{-i\varphi_n(k)}\nabla_k e^{i\varphi_n(k)}|U_{nk}\rangle$$

$$= \underbrace{-i\langle U_{nk}|\nabla_k|U_{nk}\rangle}_{=A_n} + \nabla_k\varphi_n(k)\langle U_{nk}|U_{nk}\rangle =$$

$$= A_n + \nabla_k\varphi_n(k)$$

So the Berry connection changes like a gage field in the <u>k-space</u>.

## <u>BERRY CURVATURE</u>

Recall $A$ is not observable as its value depends on the choice of a gage.
The quantity with a physical meaning is a curl of it, which is a magnetic field $B$.

$$\underline{F_n} = \nabla_k \times A_n = -i\epsilon_{ik}\partial_{k_i}\langle U_{nk}|\partial k_i|U_{nk}\rangle = \underline{-i\epsilon_{ij}\langle\partial_{k_i}U_{nk}|\partial_{k_j}U_{nk}\rangle}$$

. This value of $F_n$ ~~are~~ is known as BERRY CURVATURE which is observable.

## POSITION OPERATOR IN LATTICE.

Without lattice: $p = -i\hbar\nabla$ and $r = i\hbar\nabla_p$
what about lattice?
One can prove that for the Bloch waves

$$r = i\partial_k\delta_{n,m} - A_{m,n}$$

where $m$ and $n$ are the Band indecis and

$$A_{m,n} = -i\langle U_{m,k}|\nabla_k|U_{nk}\rangle.$$

Note if $m=n$ it turnes into the Berry connection.
if separation between bands large we can zoom in to one band and ignore many other.

$$\begin{cases} r = i\partial_k - A_n \\ p = -i\partial_r - \frac{e}{c}A \end{cases}$$

, comparing to the momentum of a charge e

→ For bloch waves the conjugate require the guige field. Berry connection is such a field.

## Berry curvature and the Hall effect.

see Haldane, Phys. Rev. Lett. 93, 206602 (2004)

In the presence of $E$ and $B$

$$\frac{dp}{dt} = F = eE + ev \times B$$

$$\frac{dr}{dt} = \nabla_p \epsilon(p) + \frac{dp}{dt} \times [\nabla_p \times A(p)]$$

$$\frac{dr}{dt} = \nabla_p \epsilon(p) + (eE + ev \times B) \times [\nabla_p \times A(p)]$$

next I will replace $p$ by $k$ $\quad p = \hbar k$

$$\frac{dr}{dt} = \frac{1}{\hbar}\{\nabla_k \epsilon(k) + (eE + ev \times B) \times [\nabla_k \times A(k)]\}$$

Recall $\quad \nabla_k \times A(k) = F(k)\bar{e}_z \quad$ where $\bar{e}_z$ is along $z$.

$$\frac{dr}{dt} = \frac{1}{\hbar}\{\nabla_k \epsilon(k) + (eE + ev \times B) \times [\nabla_k \times A(k)]\} = \frac{1}{\hbar}[\nabla_k \epsilon(k) +$$

$$+ (eE \times e_z + ev \times B \times e_z) F(k)]$$

If all electrons have the same velocity: $j = env = \frac{eNv}{A}$

But in reality for particles with different $k$ velocities are different so $Nv = \sum_{n,k} v_{n,k}$ ← all occupied states.

$$j = \frac{e}{A}\sum v_{n,k} = \frac{e}{A}\sum_{n,k}\frac{dr}{dt} = \frac{e}{A}\sum_{n,k}\frac{1}{\hbar}[\nabla_k \epsilon_n(k) +$$

$$(e\bar{E} \times e_z + ev \times B \times e_z) F_n(k)]$$

The Hall effect comes from $eE \times e_z$ as it's the only term which generates $\sigma \perp E$. And we can ignore all other terms, when we compute Hall conductivity. For Hall current $\perp E$

$$j_H = \frac{e}{A}\sum_{n,k}\frac{1}{\hbar} eE \times e_z F_n(k) = e^2 E \times e_z \frac{1}{A}\sum_{nk} F_n(k)$$

$$\sigma_{xy} = \frac{j_H}{E} = \frac{e^2}{\hbar}\frac{1}{A}\sum_{n,k} F_n(k)$$

For completely filled bands

$$\sum_{n,k} F_n(k) = A \int_{BZ} \frac{d^2k}{(2\pi)^2} F_n(k) \rightarrow$$

$$\boxed{\sigma_{xy} = \frac{j_H}{E} = \frac{e^2}{\hbar}\frac{1}{A}\sum_{nk} F_n(k) = \frac{e^2}{\hbar}\left[\int_{BZ} d^2k \frac{F_n(k)}{2\pi}\right.}$$

Notice this is when all bands are fully occupied!

# Dirac quantization, Gauss-Bonnet theorem

From math point of view $B$, Berry curvature $\mathcal{F}_n$ and the Gaussian curvature $k$ are the same!
So for simplicity we will use $B$ to calculate

— $\oiint B\,ds$ and show it's quantized.

$$\oiint B\cdot ds = \oiint B_n\,dS = \frac{c\hbar}{2q_e}\cdot n$$ , $n$ = integer magnetic charge which measures the # of magnetic monopoles inside $M$

— $\oiint k\,dS = 2\pi\chi_M$, $\chi_M$ is even integer, known as the Euler characteristic, which measures the topological nature of the manifold $M$

— $\oiint_{BZ} \mathcal{F}\,dk = 2\pi C$ quantized, $C$ is an integer called as the TKNN invariant or the Chern number

## MAGNETIC MONOPOLE AND DIRAC quantization

(see M. Nakahara, Geometry, topology and physics, IOP)

For electric charge : $q_e = \oiint_M E\cdot dS$, $\nabla\cdot E = \rho$

For magnetic field: $q_m = \oiint_M B\cdot dS$, $q_m = 0$ b/c $\nabla\cdot B = 0$

But if there is a magnetic monopole!

$$B = q_m\frac{e_r}{r^2} = q_m\frac{r}{r^3} = q_m\frac{(x,y,z)}{(x^2+y^2+z^2)^{3/2}}$$

$\nabla\times A = B$. The value of $A$ is not unique, but they are connected by a gauge transformation.

$$A = q_m\frac{(y,-x,0)}{r(r-z)} \Rightarrow \nabla\times A = q_m\nabla\times\frac{(y,-x,0)}{r(r-z)} =$$

$$q_m(\partial_x\ \partial_y\ \partial_z)\times\frac{(y,-x,0)}{r(r-z)} = \dots\dots = q_m\frac{(x,y,z)}{(x^2+y^2+z^2)^{3/2}}$$

And it's singular at $z=r$.
In fact we can prove that no matter what there will be always one singular point.
The point is $A$ is NON singular but non observable all observables are singular.

Moreover for the gauge $A = q_m\frac{(-y,x,0)}{r(r+z)}$ has a pole $z=-r$ (south pole)

$$\begin{cases} A_N = q_m\frac{(-y,x,0)}{r(r+z)} \\ A_S = q_m\,(y,-x,0)/r(r-z) \end{cases}$$

At the equator the vector potential is multivalued

i.e. $A_N = A_S + 2q_m \frac{(-y,x,0)}{(r-z)(r+z)}$ ; at $z=0$ $A_N = A_S + 2q_m \frac{(-y,x,0)}{r^2}$

$\phi \to \Phi' = \phi - \frac{\partial \Lambda(r,t)}{c\,\partial t}$ $= A_N + 2q_m \nabla\varphi$

$A \to A' = A + \nabla\Lambda(r,t)$ , $\psi(r,t) \to \psi'(r,t) = \psi(r,t)\, e^{i\frac{q_e}{c\hbar}\Lambda}$

Here $\Lambda(r,t) = 2q_m \varphi$

$\psi_N(r,t) = \psi_S(r,t)\, e^{i\frac{q_e}{c\hbar}\Lambda} = \psi_S\, e^{i\frac{2q_m q_e}{c\hbar}\varphi}$

also we know $\varphi$ and $\varphi + 2\pi$ are the same point.

$\varphi$: $\psi_N(r,t) = \psi_S(r,t)\, e^{i\frac{2q_m q_e}{c\hbar}\varphi}$

and $\varphi + 2\pi$: $\psi_N(r,t) = \psi_S(r,t)\, e^{i\frac{2q_m q_e}{c\hbar}(\varphi+2\pi)}$

to have both equations valid $\frac{2q_m q_e}{c\hbar} = n$ $\to$ $\boxed{q_m = \frac{c\hbar}{2q_e} n}$

$\psi_N = \psi_S\, e^{in(\varphi+2\pi)} = \psi_S\, e^{in\varphi}$

Why charge is quantized?

Nobody knows.

Going back to the Hall conductivity

$$\underline{\underline{\sigma_{xy}}} = \frac{e^2}{\hbar}\left[\sum_{n,\kappa\in \text{fully occupied}} \int_{BZ} d^2k\, \frac{F_n(k)}{2\pi}\right] = \underline{\underline{\frac{e^2}{\hbar} n}}$$

END OF COURSE FOR FALL 2018