Geometrical band theory and topological insulators.

4 lectures of 1,5 hours.

I. Homotopy groups & fiber bundles } background material in topology & geometry
   (topological defects) (Dirac monopole) } in order to have a common language } core/heart of the subject

II. Geometrical band theory and (Berry phases in solid state physics) }

III. TRB topological insulators : QHE and the Haldane model } two concrete examples
    ($\mathbb{Z}$)

IV. TRS topological insulator : Kane & Mele's model }
    ($\mathbb{Z}_2$)

General introduction :
(Thin message)

↗) Modern band theory : band theory is richer than previously thought
                          band theory is not only about energy bands $E_n(\vec{k})$
                          but also about Bloch functions $u_n(\vec{k})$ i.e. wavefunctions.
                          some physical quantities depend on the phase of $u_n(\vec{k})$

{ hidden geometrical structure in band theory   due to coupling
                                                 between bands
  emergent gauge field : Berry phases

[static   also quantum metric

↳ also called fiber bundle

  → geometry : local properties in $\vec{k}$ space . Anomalous velocity.

  → topology : global ——————————— . Quantum Hall effect.

2) Topological insulator : similar to the quantum Hall effect in at least three respects :
   - bulk insulator (characterized by an integer invariant)
   - conducting edge states that are robust (chiral or helical or ...)
   - bulk - edge correspondance : # of chiral edge modes
                                = change in topological invariant across
                                  the boundary

(a trivial insulator is adiabatically connected to an atomic insulator)

3) Dirac in condensed matter

   a) Dirac equation : emergent
                       as the minimal band coupling
                       quantum mechanical
                       also Jackiw-Rebbi

   b) Projection in an adiabatic/semiclassical limit [e.g. Dirac eqt in 3+1
      to Pauli eqt]
      emergent gauge field / fiber bundle [e.g. Dirac magnetic monopole]
      also Aharonov-Bohm, Berry

I. Topological defects and the Dirac monopole

During the first lecture we will review background material needed to describe geometrical/topological band Theory.

These are mathematical notions but we will use physical examples to introduce them.

A first example is homotopy groups (a notion of topology introduced by Poincaré 1895), which we will introduce via topological defects in order parameters.

A second example is fiber bundles (a notion of geometry developed by Whitney, Stiefel, Pontrjagin & Chern [30's-40's]), which we will review via the magnetic monopole of Dirac 1931.

1) Topological defects in order parameters

original works by Kléman, Toulouse, Mineev, Volovik, Mermin 1976-79

nice review by James Sethna 1991 on his website

In the realm of Landau's theory of phase transitions. In his view, different phases of matter are distinguished by different symmetries and are characterized by an order parameter (O.P.). Sethna describes Landau's theory as a four-step procedure:

① Identify the broken symmetry

② Define an O.P.

③ Study the elementary linear excitations (small oscillations of the O.P.)

④ Classify the topological defects of the O.P.

A topological defect is a singularity of the O.P. that can not be patched/repaired by any number of components of the O.P. local rearrangement.

ex:: Heisenberg $(n=3)$ ferromagnet in 3D $(d=3)$

broken symmetry = $\begin{cases} \text{space rotations } SO(3) \longrightarrow SO(2) & \text{[we are left with rotations around} \\ \text{time-reversal (TR)} & \text{the magnetization direction]} \end{cases}$

O.P. = local magnetization $\vec{M}(\vec{r})$

In the ordered phase, at low temperature $(T \ll T_c)$, the norm of the magnetization is almost constant
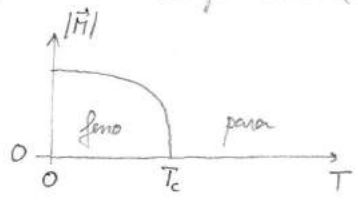
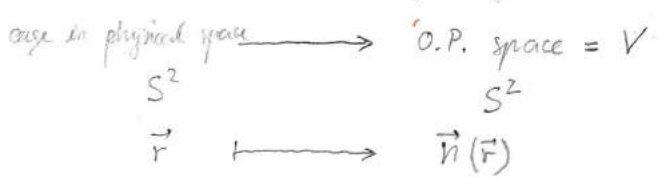Therefore $\vec{M}(\vec{r}) \simeq M_0 \, \vec{n}(\vec{r}) \in S^2$ (ie. usual sphere)

Because there is a SSB of a continuous symmetry $SO(3) \xrightarrow{SSB} SO(2)$, soft modes appear (Goldstone). There are two transverse spin waves.

What about topological defects?

To capture a d'-dim. defect ($d'=0$ is a point, $d'=1$ is a line, $d'=2$ is a plane) one needs a r-dim. cage such that
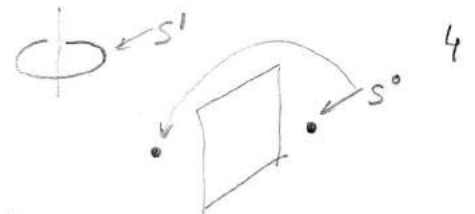
$$\boxed{1 + d' + r = d}$$ which is the counting rule (Kléman & Toulouse)

For example, in $d=3$ a point-like defect $d'=1$ require a $r=2$-dim. cage.

One therefore tries to classify maps from inequivalent

cage in physical space $\longrightarrow$ O.P. space = V

S^2 $\qquad\qquad\qquad\qquad\qquad$ S^2

$\vec{r}$ $\longmapsto$ $\vec{n}(\vec{r})$

For a line-like defect, maps $S^1 \longrightarrow S^2$

For a plane-like defect, maps $S^0 \longrightarrow S^2$

Mathematicians come to the rescue with the notion of homotopy groups (Poincaré 1895, Analysis situs).

We look for equivalence classes of (oriented loops) on manifolds. This will allow us to classify maps. We are allowed to continuously deform the loops but not to cut or glue.

examples: · $(S^1) \longrightarrow (S^1)$ circle

$$\Pi_1(S^1) = \mathbb{Z} \quad \text{ie the group } \{\mathbb{Z}; +\}$$

↑ 1st homotopy group (fundamental group)
there are as many classes as elements in $\mathbb{Z}$

· $S^1 \longrightarrow S^2$ sphere

$$\Pi_1(S^2) = 0 \quad \text{ie the trivial group } \{0; +\}$$
There is a single trivial class
"One cannot lasso a basketball."

winding number $= +2$
$W \in \mathbb{Z}$
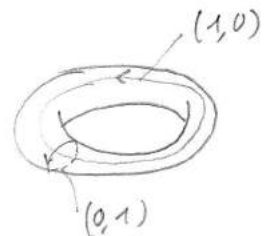first example of a topological invariant

There is no winding #

· $S^1 \longrightarrow T^2 = S^1 \times S^1$ torus

$$\Pi_1(T^2) = \mathbb{Z} \times \mathbb{Z}$$

There are two types of non-contractible loops
one needs two integers
the topological invariant here is (W_1, W_2)

$(1,0)$

$(0,1)$

· One can generalize the notion to manifolds other than S^1

$$S^2 \longrightarrow S^2$$

$$\Pi_2(S^2) = \mathbb{Z} \quad \text{mapping number}$$

↑ 2nd homotopy group

· By convention $\Pi_0(V)$ gives the number of connex components of V.
It is not a group.

$\Pi_0(SO(3)) = 0$ 1 component
$\Pi_0(O(3)) = \mathbb{Z}_2$ 2 components
$\Pi_0(S^1) = 0$ 1 component
$\Pi_0(S^0) = \mathbb{Z}_2$ 2 components
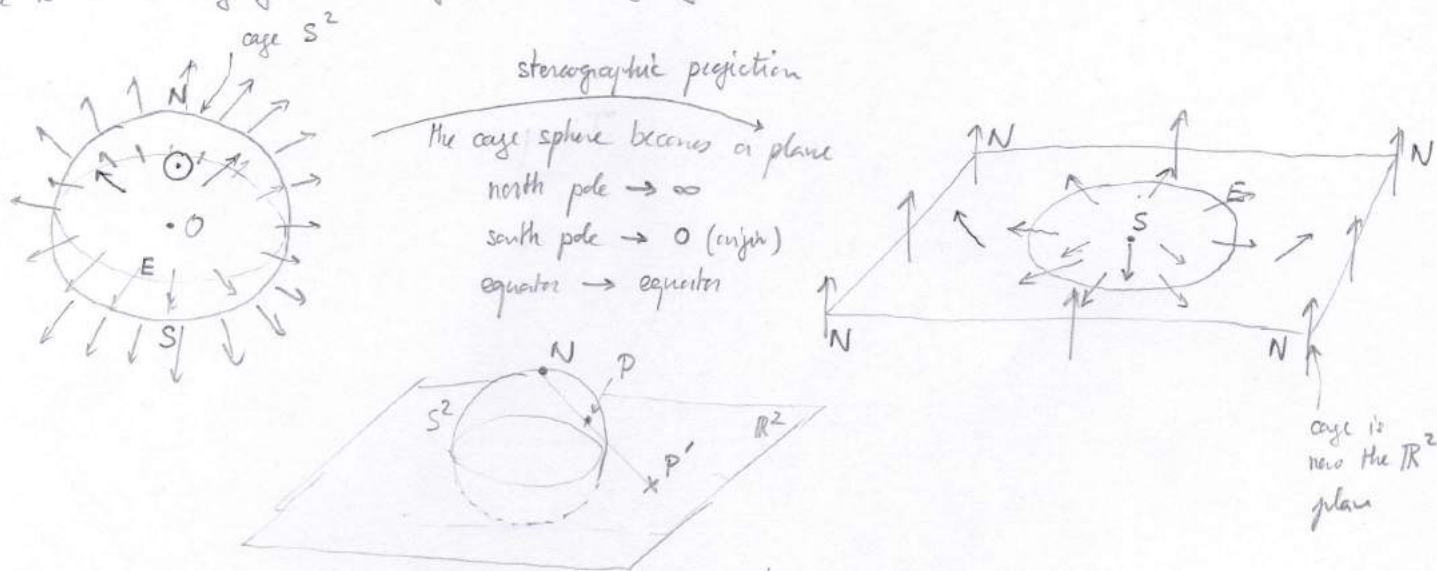
$S^0 = 2$ points

Back to the Heisenberg ferromagnet with $V = S^2$ as $\vec{M}(\vec{r}) \simeq M_0 \vec{n}(\vec{r})$

as $\quad \Pi_0(S^2) = 0 \quad$ no topological plane-like defect (domain wall)

$\Pi_1(S^2) = 0 \quad$ ———————— line ————————

$\Pi_2(S^2) = \mathbb{Z} \quad$ topological point-like defects classified by a mapping number. These are known as <u>hedgehogs</u> (and have a close relationship to baby-skyrmions) or <u>Bloch points</u>.

Here is a drawing of the charge $+1$ hedgehog:

stereographic projection

the cage sphere becomes a plane
north pole $\to \infty$
south pole $\to 0$ (origin)
equator $\to$ equator

cage is now the $\mathbb{R}^2$ plane

do not confuse this with a (baby) skyrmion which is a 2D topological texture and not a 3D topological defect.

remark: domain walls are stable <u>topological textures</u> (soliton configurations) in 3D Heisenberg ferromagnets. They are not defects (no singularity) and require imposed boundary conditions for their existence.

Summary: homotopy groups allow me to think of topological defects
to classify them
to characterize them with integers (known as topological invariants)

stability of topological defects
topological invariants are useful to study the creation/annihilation of topological defects (think of the $+1$ and -1 vortices of the Kosterlitz-Thouless transition for 2D XY model ie. $d=2$ and $n=2$).

2) Dirac's magnetic monopole and fiber bundles

Dirac 1931: electromagnetism and quantum mechanics permit the existence of a quantized magnetic monopole.

Hopf 1931: Hopf fibration, an example of fiber bundle

a) Quantum mechanics in the presence of a vector potential $\vec{A}$

minimal coupling : $\vec{P} \rightarrow \vec{P} - q\vec{A} = \vec{P} - e\vec{A}$ for a charged particle with electric charge $q = +e$

ie. $\vec{\nabla} \rightarrow \vec{\nabla} - i\frac{e}{\hbar}\vec{A} \equiv \vec{D}$

↑ derivative   ↑ connection   ↑ covariant derivative $\vec{B} = \vec{\nabla} \times \vec{A}$ is the __curvature__

for the wavefunction, it means $\psi(\vec{r}) \rightarrow \psi(\vec{r}) e^{+i\frac{e}{\hbar}\int^{\vec{r}} d\vec{\ell}\cdot\vec{A}}$

phase $\theta(\vec{r})$ U(1)

__Aharonov-Bohm phase__ : after parallel transport along a closed path, the wavefunction comes back to itself up to a non-integrable phase (also known as a geometric phase or anholonomy)

$e^{i\Gamma_{AB}} = e^{i\frac{e}{\hbar}\oint_{\mathcal{C}} d\vec{\ell}\cdot\vec{A}} = e^{i\frac{e}{\hbar}\int_{S} d^2\vec{S}\cdot\vec{B}} = e^{i\frac{e}{\hbar}\phi}$ magnetic flux

$\frac{e}{\hbar}\phi$ is a phase, an angle : it matters modulo 2π

$\Rightarrow \phi$ matters modulo $\frac{h}{e} \equiv \phi_0$: __magnetic flux quantum__ (this is already an addition to Maxwell's electromagnetism)

A gauge transform is a dble transformat°:

. on the vector potential $\vec{A} \rightarrow \vec{A}' = \vec{A} + \vec{\nabla}\chi$ already in classical electromagnetism (but $\vec{B}$ is unchanged)

. on the wavefunction $\psi(\vec{r}) \rightarrow \psi'(\vec{r}) = \psi(\vec{r}) e^{i\frac{e}{\hbar}\chi(\vec{r})}$ in QM

$\theta(\vec{r})$

It is a __U(1)__ phase transformation.

b) Magnetic monopole of charge g at $\vec{r} = 0$

$$\vec{\nabla} \cdot \vec{B} = g\,\delta(\vec{r}) \qquad \text{instead of } 0$$

$$\vec{B} = \frac{g}{4\pi} \frac{\vec{r}}{r^3} \qquad \text{singularity of } \vec{B} \text{ at } \vec{r} = 0$$

Is this possible?

What is the flux across a sphere S^2?

$$\phi = \int_{S^2} d^2\vec{S} \cdot \vec{B} = \int_{Volume} d^3r \underbrace{(\vec{\nabla} \cdot \vec{B})}_{g\,\delta(\vec{r})} = g$$

If there exists a smooth global gauge (i.e. $\vec{A}$ is well defined over all S^2 and such that $\vec{B} = \vec{\nabla} \times \vec{A}$) then Stokes' theorem is applicable and

$$\phi = \int_{S^2} d^2\vec{S} \cdot \vec{B} = \int_{S^2} d^2\vec{S} \cdot (\vec{\nabla} \times \vec{A}) = \oint_{\partial S^2} d\vec{\ell} \cdot \vec{A} = 0 \qquad \text{as } \partial S^2 = 0.$$
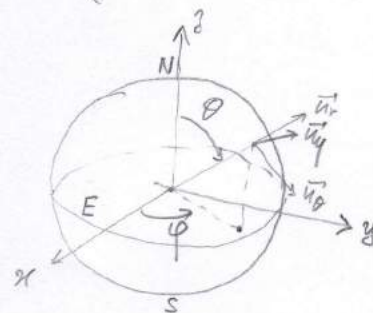
$\Rightarrow$ if $g \neq 0$ then there exist no smooth gauge!

Wu & Yang 1975 introduced the idea of having patches for $\vec{A}$ and a gauge transformation to connect the patches.

North hemisphere: $\quad \vec{A}^N = \frac{g}{4\pi} \frac{1-\cos\theta}{r\sin\theta}\,\vec{u}_\varphi$

well-defined at N $\quad (\vec{A}^N = 0)$
ill-_____ S $\quad (\vec{A}^S \to \infty)$

South hemisphere: $\quad \vec{A}^S = \frac{g}{4\pi} \frac{-1-\cos\theta}{r\sin\theta}\,\vec{u}_\varphi$

ill-defined at N
well _____ S

$$\vec{B}^N = \frac{g}{4\pi} \frac{\vec{u}_r}{r^2} + g\,\delta(x)\,\delta(y)\,\Theta(-z)\,\vec{u}_z$$
$$\vec{\nabla} \cdot \vec{B}^N = 0$$

On most of $\mathbb{R}^3$, $\vec{B}^N = \vec{B}^S$; but they disagree along $z < 0$ and $z > 0$. Therefore, there exist no gauge transformation on all of $\mathbb{R}^3$ that transforms $\vec{A}^N$ into $\vec{A}^S$.

However $\vec{B}^N = \vec{B}^S$ on the equator.

$$\vec{A}^N - \vec{A}^S = \frac{g}{2\pi r\sin\theta}\,\vec{u}_\varphi = \vec{\nabla}\chi \quad \text{with} \quad \chi = \frac{g}{2\pi}\varphi$$

as $\quad \vec{\nabla}\chi = \frac{\partial\chi}{\partial r}\,\vec{u}_r + \frac{1}{r}\frac{\partial\chi}{\partial\theta}\,\vec{u}_\theta + \frac{1}{r\sin\theta}\frac{\partial\chi}{\partial\varphi}\,\vec{u}_\varphi$

The total flux across the sphere is:

$$\phi = \int d^2\vec{S} \cdot \vec{B} = \int_N d^2\vec{S} \cdot (\vec{\nabla}\times\vec{A}^N) + \int_S d^2\vec{S}\cdot(\vec{\nabla}\times\vec{A}^S) = \oint_E d\vec{\ell}\cdot\vec{A}^N - \oint_E d\vec{\ell}\cdot\vec{A}^S$$

$$= \oint_E d\vec{\ell}\cdot\vec{\nabla}\chi = \frac{g}{2\pi}\oint_E d\varphi = g \qquad \text{OK. This means that } \vec{\nabla}\cdot\vec{B} = g\,\delta(\vec{r}) \text{ with } \vec{B} \text{ built from}$$

the two patches $\vec{A}^N$ and $\vec{A}^S$.

But χ is also changing the phase of the wf during the gauge transformation:

$$\begin{cases} \vec{A}^S \rightarrow \vec{A}^N = \vec{A}^S + \vec{\nabla}\chi \\ \psi^S(\vec{r}) \rightarrow \psi^N(\vec{r}) = \psi^S(\vec{r})\, e^{i\frac{e}{\hbar}\chi(\vec{r})} = \psi^S(\vec{r})\, e^{i\frac{g}{\phi_0}\varphi} \end{cases}$$

$\theta = \pi/2$

And the wf has to be single-valued ie.

$$\psi^N(r, \theta=\tfrac{\pi}{2}, \varphi+2\pi) = \psi^N(r, \theta=\tfrac{\pi}{2}, \varphi) \quad \text{and} \quad \psi^S(r, \theta=\tfrac{\pi}{2}, \varphi+2\pi) = \psi^S(r, \theta=\tfrac{\pi}{2}, \varphi)$$

$$\Rightarrow \quad e^{i\frac{g}{\phi_0}(2\pi+\varphi)} = e^{i\frac{g}{\phi_0}\varphi} \quad \text{ie.} \quad e^{i\,2\pi\frac{g}{\phi_0}} = 1$$

$$\boxed{g = \text{integer} \times \phi_0}$$

A magnetic monopole is permible but its charge should be quantized.
The wavefunction along the equator is actually a wave-section.
remark: • a _non-zero monopole charge_ can be seen as _an obstruction to finding a smooth global gauge_.

• total flux across the sphere

$$\frac{\phi}{\phi_0} = \frac{1}{\phi_0}\int_{S^2} d^2\vec{S}\cdot\vec{B} = \frac{g}{\phi_0} = \text{integer} \in \mathbb{Z}$$

if ϕ matters modulo ϕ_0 then a quantized magnetic monopole is the modulus

These two features will be encountered later when discussing Chern numbers.
Rk: $\vec{A}$ is more fundamental than $\vec{B}$ even if $\vec{A}$ is gauge-dependent and $\vec{B}$ is gauge-invariant.

c) <u>The Wu & Yang dictionary : from gauge fields to fiber bundles</u>

There is a mathematical (geometrical) notion hidden here. It is that of fiber bundles.
Wu & Yang 1975 understood that gauge fields (in physics) = fiber bundles (in maths).

electromagnetism	fiber bundle (a U(1) complex vector bundle)
$\vec{A}$ vector potential	connection (describes parallel transport)
$\vec{B}$ magnetic field	curvature
Γ_{AB} AB phase	anholonomy (in parallel transport) geometric phase
Dirac's monopole quantization	classification of U(1) bundles according to the 1st Chern number
$-i\hbar\vec{\nabla} - e\vec{A}$ minimal coupling	covariant derivative
$\psi^N(\vec{r}) = \psi^S(\vec{r})e^{i\frac{g}{\phi_0}\varphi}$ wavefunction on the equator region (integer)	section (rather than a function)

after the Möbius strip.

Fiber bundle is a notion of geometry (~ Whitney 1930's)

a fiber bundle E ~~compact~~

consists of a base space B (a manifold) e.g. S^1
and of a fiber F e.g. $\mathbb{R}$ or a segment $[0,1]$ or S^1

a projection map $p: E \longrightarrow B$

$$F \hookrightarrow E \xrightarrow{P} B$$

| locally E looks like $B \times F$ but not necessarily globally |

a structure group G can act on the fiber (e.g. $G = U(1)$ if $F = S^1$)

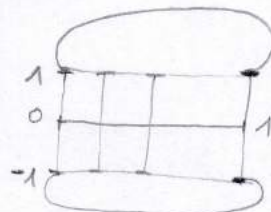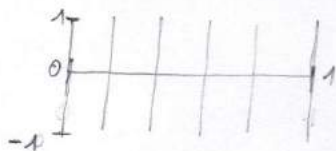if globally $E = B \times F$ the bundle is said to be trivial

if ~~globally~~ $E \neq B \times F$ ————————————————— twisted or non-trivial.

A twisted fiber bundle is characterized by topological invariants (called characteristic classes).
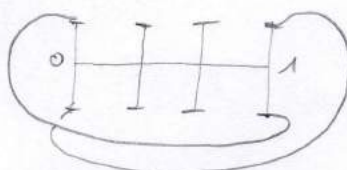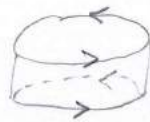The most famous is the Chern number.

ex: Möbius strip   (Möbius ; Listing 1858)

$B = S^1$ (first $[0, 2\pi]$ and then S^1)
$F = [-1, 1]$ and then S^1

cylinder
$E = B \times F$
trivial bundle

Möbius strip
twisted bundle
$E \neq B \times F$

a single edge and
a single side
(non-orientable)

other similar example is the Klein bottle vs the torus with $B = S^1$ and $F = S^1$

$$T^2 = S^1 \times S^1$$

Back to the Dirac monopole : $B = S^2$ (as $\mathbb{R}^3 \setminus \{0\} = S^2 \times \mathbb{R}^{+*} \sim S^2$)
Hopf bundle, fibration $F = S^1$ (is the phase)
                               $G = U(1)$ (is the gauge freedom)

$$S^1 \hookrightarrow E \xrightarrow{P} S^2$$
$$\underset{\shortparallel}{}$$
$$S^3$$

Is this bundle twisted ?
- No global section ie. obstruction
- The answer is contained in the Chern number :
 (This is also the charge of the monopole)

$$C = \frac{1}{\phi_0} \int_{S^2} d^2\vec{S} \cdot \vec{B} = \frac{g}{\phi_0} = \text{integer} \neq 0$$

curvature   ie. $\vec{B} = \frac{C}{2} \frac{\vec{r}}{r^3}$

remark: this is not the same as a point-like
topological defect in a 3D superfluid for
which $d = 3$, $n = 2$, $V = S^1$ and

$$\pi_2(S^1) = 0$$

Hopf invariant classifies maps $S^3 \to S^2$

$$\pi_3(S^2) = \mathbb{Z}$$