$$j_H = \frac{e^2}{2\pi h} \sum_{n \text{ fully occupied bands}} \int_{BZ} d\vec{k}\, \vec{E} \times \left[\vec{\nabla}_k \times \vec{\mathcal{A}}_n(k)\right] = \vec{E} \times \left[\frac{e^2}{h} \frac{1}{2\pi} \sum_{n \text{ fully occupied bands}} \int_{BZ} d\vec{k}\, \vec{E} \times \vec{\mathcal{F}}_n(k)\right] \tag{3.121}$$

$$\sigma_{xy} = \frac{e^2}{h} \sum_{n \text{ fully occupied bands}} \left[\frac{1}{2\pi} \int_{BZ} d\vec{k}\, \vec{\mathcal{F}}_n(k)\right] \tag{3.122}$$

In the next section, we will show that the integral here is always an integer, and it is a topological index.

From now on, I will use the theorist's unit: $k_B = e = c = h = \hbar = 2\pi = 1$ so

$$\sigma_{xy} = \sum_n \left[-\frac{i}{2\pi} \int_{BZ} d\vec{k}\, \epsilon_{ij} \langle \partial_{ki} u_{n,k} \mid \partial_{kj} u_{n,k} \rangle\right] \tag{3.123}$$

is just an integer.

3.7. Dirac Quantization, Gauss– Bonnet theorem and the TKNN (Thouless —Kohmoto —Nightingale —den Nijs) Invariant

From the mathematical point of the view, the following three objects are the same thing (fiber bundles): the magnetic field B, the Berry curvature $\mathcal{F}$, and the Gaussian curvature of K (geometry). All of them are described by the same mathematical structure: fiber bundles.

In the next a few sections, we will investigate the integral of B, $\mathcal{F}$ and K on a closed 2D manifold. (close: no boundary). And shows that they are all quantized due to topological reasons, which is known as topological quantization.

$$\oiint_M B \cdot dS = \oiint_M B_n\, dS = \frac{c\hbar}{2 q_e} n \qquad \text{quantized}: n \text{ is an integer,} \tag{3.124}$$

known as the magnetic charge, which measures the number of magnetic monopole inside M

$$\oiint_M K\, dS = 2\pi \chi_M \qquad \text{quantized}: \chi_M \text{ is an even integer,} \tag{3.125}$$

known as the Euler characteristic, which measures the topological nature of the manifold M

$$\oiint_{BZ} \mathcal{F}\, d\vec{k} = 2\pi C \qquad \text{quantized}: C \text{ is an integer,} \tag{3.126}$$

known as the TKNN invariant or the Chern number, which measures the quantized Hall conductivity for a topological insulator

3.8. Magnetic monopole and Dirac quantization condition

Reference: M Nakahara, Geometry, topology and physics, IOP

For electric charge, the Gauss's law tell us that

$$q_e = \oiint_M E \cdot dS \tag{3.127}$$

In Maxwell's equations, this is:

$$\nabla \cdot E = \rho \tag{3.128}$$

For magnetic fields, we can do the same thing:

$$q_m = \oiint_M B \cdot dS \tag{3.129}$$

Without magnetic monopoles, $q_m = 0$, because $\nabla \cdot B = 0$

Assume that there is a magnetic monopole with charge q_m, what will happen?

The B fields is:

$$\vec{B} = q_m \frac{\vec{e}_r}{r^2} = q_m \frac{\vec{r}}{r^3} = q_m \frac{(x,\ y,\ z)}{(x^2 + y^2 + z^2)^{3/2}} \tag{3.130}$$

What about the vector potential? $\vec{A} = ?$

$$\nabla \times \vec{A} = \vec{B} \tag{3.131}$$

The value of $\vec{A}$ is not unique, but they are all connected by a gauge transformation.

$$\vec{A} = q_m \frac{(y,\ -x,\ 0)}{r(r-z)} \tag{3.132}$$

$$\begin{aligned}
&\nabla \times \vec{A} = q_m \nabla \times \frac{(y,\ -x,\ 0)}{r(r-z)} = \\
&q_m(\partial_x,\ \partial_y,\ \partial_z) \times \frac{(y,\ -x,\ 0)}{r(r-z)} = q_m\left(\partial_y \frac{0}{r(r-z)} - \partial_z \frac{-x}{r(r-z)},\ \partial_z \frac{y}{r(r-z)} - \partial_x \frac{0}{r(r-z)},\ \partial_x \frac{-x}{r(r-z)} - \partial_y \frac{y}{r(r-z)}\right) = \\
&q_m\left(-\partial_z \frac{-x}{r(r-z)},\ \partial_z \frac{y}{r(r-z)},\ \partial_x \frac{-x}{r(r-z)} - \partial_y \frac{y}{r(r-z)}\right) = q_m \frac{(x,\ y,\ z)}{(x^2 + y^2 + z^2)^{3/2}}
\end{aligned} \tag{3.133}$$

This vector potential has one problem. It is singular at the north pole ($z = r$). In fact, one can prove that no matter which gauge one uses, there will always be a singularity point.

Here, I must emphasize that this singularity is not a physical singularity. All physical observables are smooth and non-singular functions at this point. Only A (which is not a measurable quantity) shows singular behavior. In addition, the location of this singularity point is gauge dependent.

For example, we can use another gauge $\vec{A}$, which gives exactly the same B field.

$$\vec{A} = q_m \frac{(-y,\ x,\ 0)}{r(r+z)} \tag{3.134}$$

This A is singular at the south pole $z = -r$.

So, we can use the first one to describe the south hemisphere and the second one to describe the north hemisphere:

$$\vec{A}_N = q_m \frac{(-y,\ x,\ 0)}{r(r+z)} \tag{3.135}$$

$$\vec{A}_S = q_m \frac{(y,\ -x,\ 0)}{r(r-z)} \tag{3.136}$$

At the equator, the vector potential is multivalued (depending on whether we use A_N or A_S), but this is not a problem. Because we know that A is not a physical observable and it IS multivalued. As long as they differ by a gauge transformation, they describe the same physics (same B field). This is indeed the case here: the gauge transformation between A_N and A_S is:

$$\vec{A}_N = \vec{A}_S + 2\, q_m \frac{(-y,\ x,\ 0)}{(r-z)\,(r+z)} \tag{3.137}$$

At equator: z=0

$$\vec{A}_N = \vec{A}_S + 2\, q_m \frac{(-y,\ x,\ 0)}{r^2} = \vec{A}_N + 2\, q_m \nabla \varphi \tag{3.138}$$

$$\Phi \to \Phi' = \Phi - \frac{\partial \Lambda(r,\ t)}{c\, \partial t} \tag{3.139}$$

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla \Lambda(r,\ t) \tag{3.140}$$

$$\Psi(r,\ t) \to \Psi'(r,\ t) = \Psi(r,\ t) \exp\left(i \frac{q_e}{c\, \hbar} \Lambda\right) \tag{3.141}$$

Here

$$\Lambda(r,\ t) = 2\,q_m\,\varphi \tag{3.142}$$

$$\Psi_N(r,\ t) = \ \Psi_S(r,\ t)\exp\left(i\,\frac{q_e}{c\,\hbar}\,\Lambda\right) = \Psi_S(r,\ t)\exp\left[i\,\frac{2\,q_m\,q_e}{c\,\hbar}\,\varphi\right] \tag{3.143}$$

We know that φ and $\varphi + 2\,\pi$ are the same point.

at φ we have:

$$\Psi_N(r,\ t) = \ \Psi_S(r,\ t)\exp\left[i\,\frac{2\,q_m\,q_e}{c\,\hbar}\,\varphi\right] \tag{3.144}$$

at $\varphi + 2\,\pi$ we have:

$$\Psi_N(r,\ t) = \ \Psi_S(r,\ t)\exp\left[i\,\frac{2\,q_m\,q_e}{c\,\hbar}\,(\varphi + 2\,\pi)\right] \tag{3.145}$$

To have both the two equations valid, $\frac{2\,q_m\,q_e}{c\,\hbar}$ must be an integer n

$$\Psi_N(r,\ t) = \ \Psi_S(r,\ t)\exp\left[i\,n\,(\varphi + 2\,\pi)\right] = \Psi_S(r,\ t)\exp(i\,n\,\varphi) \tag{3.146}$$

This tells us that the magnetic charge is quantized:

$$q_m = \ \frac{c\,\hbar}{2\,q_e}\,n \tag{3.147}$$

Q: Why charge are quantized in our universe?

A: Unknown. It is still a mystery. But, if we can find even a single magnetic monopole somewhere in our universe, the Dirac quantization condition immediately solves this puzzle for us.

$$q_e = \frac{c\,\hbar}{2\,q_m}\,n \tag{3.148}$$

For a closed surface enclosing a magnetic monopole, no matter what gauge one uses, the vector potential must have some singularities.

If A is a non-singular function on a closed manifold, the magnetic flux through this manifold must be zero.

To proof this, we cut the manifold into two parts D_I and D_{II}

The magnetic flux though D_I is

$$\int\int_{D_I} d\,S\cdot B = \int\int_{D_I} d\,S\cdot\nabla\times A = \int_{\partial D_I} d\,l\cdot A \tag{3.149}$$

Here we use the Stokes' theorem and $\partial\,D_I$ is the edge of D_I.

The magnetic flux though D_{II} is

$$\int\int_{D_{\text{II}}} d\,S\cdot B = \int\int_{D_{\text{II}}} d\,S\cdot\nabla\times A = \int_{\partial D_{\text{II}}} d\,l\cdot A \tag{3.150}$$

Therefore, the total magnetic field flux is

$$\oint\!\!\!\oint_M B\cdot d\,S = \int\int_{D_I} d\,S\cdot B + \int\int_{D_{\text{II}}} d\,S\cdot B = \int_{\partial D_I} d\,l\cdot A + \int_{\partial D_{\text{II}}} d\,l\cdot A \tag{3.151}$$

Notice that the edge of D_I and D_{II} are the same curve but their directions are opposite.

$$\partial\,D_I = -\partial\,D_{\text{II}} \tag{3.152}$$

$$\oint\!\!\!\oint_M B\cdot d\,S = \int_{\partial D_I} d\,l\cdot A - \int_{\partial D_I} d\,l\cdot A = 0 \tag{3.153}$$

The only way to have nonzero magnetic flux here is to have some singular vector potential. If A is singular (for all any gauge choice), we must use at least two different gauge choice to cover the whole manifold.

If we use A_I for D_I uses A_{II} for D_{II}, we get

$$\oiint_M B \cdot dS = \int_{\partial D_I} dl \cdot A_I - \int_{\partial D_I} dl \cdot A_{\text{II}} = \int_{\partial D_I} dl \cdot (A_I - A_{\text{II}}) \tag{3.154}$$

Here, I emphasize again that this singularity in A is not a physical singularity. It you measure any physical observables, there is nothing singular here. The singularity lies in A, which is NOT a physical observable. The location of this singularity changes when one choose another gauge. But no matter how one choose the gauge, there must be at least one singularity.

Later we will show that the same conclusion holds for the Berry curvature. For insulators, if the Bloch wavefunction can be defined for any k in the BZ without singularity. We can show that

$$\oiint_{\text{BZ}} \mathcal{F}\, d\vec{k} = \int_{\partial D_I} dl \cdot \mathcal{A} - \int_{\partial D_I} dl \cdot \mathcal{A} = 0. \tag{3.155}$$

Since this integral is the Hall conductivity, this means that $\sigma_{\text{xy}} = 0$ if the Bloch wave function can be defined at any k without singularity.

To have nonzero Hall conductivity, the Bloch wave functions must have some singular point in the k-spaces. As a result, we will need to define different Bloch wave functions for different regions of the k-space and these Bloch waves are connected by a gauge transformation at the boundary.

$$\left| u^{\text{II}}{}_{n,k} \right\rangle = e^{i\,\phi_n(k)} \left| u^{I}{}_{n,k} \right\rangle \tag{3.156}$$

We know that the Berry connection changes under this phase shift, so the Berry connections in the different regions must be different also

$$\vec{\mathcal{A}}^{\text{II}}{}_n = \vec{\mathcal{A}}_n{}^I + \nabla_{\vec{k}}\, \phi_n(k) \tag{3.157}$$

This singularity again is not a physical singularity. All physical observables show no singular behavior and their values are continuous function of k, when we go across the boundary for these different regions. The discontinuities and singularities can only be seen when you look at quantities that cannot be measured, like the phase of a wavefunction and the Berry connection. Because we use different $\mathcal{A}$ for different regions, we have

$$\oiint_{\text{BZ}} \mathcal{F}\, d\vec{k} = \int_{\partial D_I} dl \cdot (\mathcal{A}_I - \mathcal{A}_{\text{II}}) \tag{3.158}$$

which could be none zero.

The quantization of the flux is only true for a closed manifold (e.g. a sphere). For a open manifold with boundaries, the flux is in general unquantified (e.g. part of a sphere).

The same is true for the Berry curvature. Only if the integral is over the whole BZ, the total Berry curvature is quantized. In other words, the Berry curvature for insulator is quantized. But for metal, it is not.

3.9. Gauss– Bonnet theorem and topology

The idea of topology originates from geometry in the descriptions of manifolds in a 3-dimensional space. Later, it is generalized other dimensions and generic abstract space (including the Hilbert space in quantum physics).

In geometry, if an manifold A can be adiabatically deformed into B, we said that they have the same topology. Otherwise, we say that they are topologically different.

Examples: the surface of a sphere and the surface of a cube are topologically equivalent.

the surface of a sphere and the surface of donut (torus) are topologically different.

To distinguish different manifolds, mathematicians developed an object, which is called an “index” (topological index). It is a number. For objects with the same topology, the index takes the same value. Otherwise, the value will be different. For 2D closed manifold, the index is the Euler characteristic:

$$\oiint_M K\, dS = 2\pi\, \chi_M \tag{3.159}$$

To define the curvature for a curve, we use a circle to fit the curve around one point on the curve. The inverse radius κ=1/R gives us the curvature.

For a manifold, one can draw lots of curves at one point. And one can get the curvature for all of these curves. Among all these curvatures, the largest and smallest one are known as principle curvatures κ_1 and κ_2. The Gaussian curvature is the product of they two.

For a sphere, $\kappa_1 = \kappa_2 = 1/R$, so $K = \frac{1}{R^2}$

For a saddle point, the surface curves up along one direction and curves down along another direction, $\kappa_1 > 0$ and $\kappa_2 < 0$. So $K = \kappa_1 \kappa_2 < 0$.

For any 2D closed manifold, the integral of $\oiint_M K \, dS$ is always an even integer and it value is invariant no matter how one deform the manifold (adiabatically).

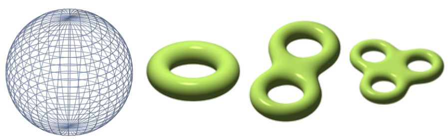
χ_M only cares about the topology of the manifold M. If we deform any manifold adiabatically (not changing the topology), χ_M will remain the same. If one change the topology, χ_M takes *a* different value.

Sphere : $\chi_M = 2$

Torus : $\chi_M = 0$

double torus : $\chi_M = -2$

triple torus : $\chi_M = -4$



figures from wikipedia.org From left to right: sphere, torus, double torus and triple torus.

Again, it is important to emphasize here that this integral is a topological index, only if we are considering a closed manifold which has no boundary. Otherwise, it is not quantized and it is not a topological index.

3.9.1. connections to other topological properties

Topology and handles

χ_M is directly related to the genus g of the manifold.

$$\chi_M = 2(1-g). \tag{3.160}$$

The genus measure the number of “handles” on a object. A sphere has no Handel, so $g = 0$. For torus g=1. For double torus g=2.

A coffee mug has one Handel. So a coffee mug is a torus from the topological point of the view. I.e. a coffee mug=a donut

Similarly, a sippy cup=a double torus (two handles)

a three-handled cup=a pretzel=a triple torus (three hazels)

χ_M and polyhedrons

Another definition of χ_M, if we draw a grid on the manifold,

$$\chi_M = V - E + F \tag{3.161}$$

where V, E, and F are the numbers of vertices (corners), edges and faces respectively.

For most polyhedron we are familiar with (simply connected polyhedron), they are topologically equivalent to a sphere, which has $\chi_M = 2$. So, these polyhedrons has

$$V - E + F = 2 \tag{3.162}$$

Topology and hair vortex

If we drop a (in-plane) vector at each point on this manifold, we get a vector fields, which may have vortices.

For a vortex, we can define its vorticity, which is an integer.

The total vorticity is χ_M

$$\chi_M = \sum v \tag{3.163}$$

For sphere $\chi_M = 2$, which means that total vorticity must be 2, which is nonzero!

One can’t comb the hair on a 2-sphere without singularities (vortex).

If one think hair as vector fields (pointing from the end to the tip), on a sphere, this hairs must have some vortex, and the total vorticity is 2.

Examples: If one comb the hair along the longitude (or latitude) directions , there are two +1 vortex at north and south poles.

If one assumes that human hair covers the north hemisphere (of the head) and pointing downward (to -z) at the equation, which is typically try for human hairs, vorticity total is +1 (half of +2). For the majority of human beings, there is one +1 vortex. But there are more complicated cases, for example two +1 and one -1, or three +1 and two -1.

3.10. Topological index for an insulator

The topological index

$$C = \frac{1}{2\pi} \sum_n \oiint_{\text{BZ}} \mathcal{F}\, d\vec{k} \tag{3.164}$$

This integral is a topological index only if we integrate $\mathcal{F}$ over the whole BZ (a closed manifold). Because a BZ has periodic boundary conditions along x and y (for a 2D system), the BZ is a torus which is a closed manifold.

$$\mathcal{F}_n\left(\vec{k}\right) = \epsilon_{\text{ij}} \left\langle \partial_{\text{ki}} u_{n,k} \,\middle|\, \partial_{\text{kj}} u_{n,k} \right\rangle \tag{3.165}$$

$$\sigma_{\text{xy}} = \frac{e^2}{h} \sum_{n,\text{ valence bands}} \left[\frac{1}{2\pi} \int_{\text{BZ}} d\vec{k}\, \mathcal{F}_n\left(\vec{k}\right)\right] + \frac{e^2}{h} \sum_{n,\text{ conduction bands}} \left[\frac{1}{2\pi} \int_{\epsilon_k<\epsilon_F} d\vec{k}\, \mathcal{F}_n\left(\vec{k}\right)\right] \tag{3.166}$$

For 2D systems, we will show below that the first term is quantized and is topologically invariant. The second term is not quantized and is not topologically invariant.

For insulators (first term only), the Hall conductivity is a topological index and is an Integer due to topological quantization.

For metals, the integral for the conducting band is take over only part of the BZ (the filled states, or say the Fermi sea). It is not quantized and it is not a topological index.

In other words, $\mathcal{F}$ gives us 2D topological insulators, but no topological metals.

3.11. Second quantization

3.11.1. wave functions for indistinguishable particles

Second quantization is a technique to handle indistinguishable particles.

Two distinguishable particles: particle one on state ψ_1 and particle two on state ψ_2

$$\Psi(r_1, r_2) = \psi_1(r_1)\, \psi_2(r_2) \tag{3.167}$$

n distinguishable particles:

$$\Psi(r_1, r_2, r_3, \ldots, r_N) = \psi_1(r_1)\, \psi_2(r_2) \ldots \psi_n(r_n) \tag{3.168}$$

Two indistinguishable particles: particle one on state ψ_1 and particle two on state ψ_2

$$\Psi(r_1, r_2) = \pm \Psi(r_2, r_1) \tag{3.169}$$

$$\Psi(r_1, r_2) = \psi_1(r_1)\, \psi_2(r_2) \pm \psi_2(r_1)\, \psi_1(r_2) \tag{3.170}$$

3 indistinguishable particles:

$$\begin{aligned}\Psi(r_1, r_2, r_3) = {} & \psi_1(r_1)\, \psi_2(r_2)\, \psi_3(r_3) \pm \psi_1(r_1)\, \psi_3(r_3)\, \psi_2(r_2) \pm \psi_2(r_2)\, \psi_1(r_1)\, \psi_3(r_3) + \\ & \psi_3(r_3)\, \psi_1(r_1)\, \psi_2(r_2) + \psi_2(r_2)\, \psi_3(r_3)\, \psi_1(r_1) \pm \psi_3(r_3)\, \psi_2(r_2)\, \psi_1(r_1)\end{aligned} \tag{3.171}$$

n indistinguishable particles:

$$\Psi(r_1, r_2, r_3, \ldots, r_n) = \sum_{\mathcal{P}} (\pm 1)^{\mathcal{P}}\, \psi_{i_1}(r_1)\, \psi_{i_2}(r_2) \ldots \psi_{i_n}(r_n) \tag{3.172}$$

where $\mathcal{P}$ represents all permutations and there are n! terms here. For large n, this is an extremely complicated wavefunction. For even ten particles, n=10, there are 2.6 million terms.