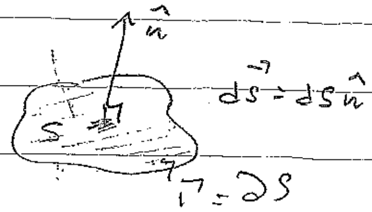
Lecture 19/11 (I.11a.

CHERN THEOREM

Last week I derived the basic "Berryology" formulas

$$\phi = \oint_\Gamma \vec{A}(\vec{\lambda})\cdot d\vec{\lambda}$$

$$\overset{2D}{=} \int_S \vec{\tilde{F}}(\vec{\lambda})\cdot d\vec{S}$$



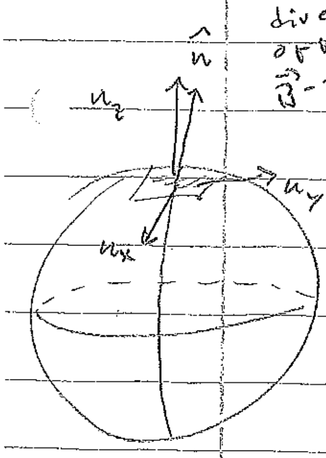
where $\vec{A} = \langle u_{\vec{\lambda}} | i\nabla_{\vec{\lambda}} | u_{\vec{\lambda}}\rangle \xrightarrow{\text{GAUGE TRANSFORMATION}} \vec{A}' = \vec{A} + \nabla_{\vec{\lambda}}\beta$

GAUGE INVARIANT $\vec{\tilde{F}} = \nabla_{\vec{\lambda}} \times \langle u_{\vec{\lambda}} | i\nabla_{\vec{\lambda}} | u_{\vec{\lambda}}\rangle \rightarrow \vec{\tilde{F}}$

Let's now go back to the example of a spinor subject to a magnetic field, but now doing the analysis in the continuum using the Berry curvature: First recall that on the Bloch sphere

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

direction of the $\vec{B}$-field

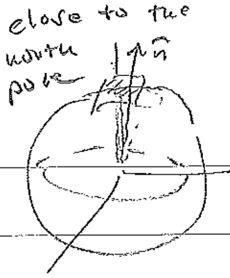


Note the implicit gauge choice in this representation: $|\uparrow_{\hat{n}}\rangle$ is smooth and continuous everywhere on the Bloch sphere except at the south pole ($\theta = \pi$) where $|\uparrow_{\hat{n}}\rangle$ has a singular dependence on φ ("vortex"). Cf. the "Dirac string"!

Close to the north pole ($\theta = 0$) we can parameterize $|\uparrow_{\hat{n}}\rangle$ using $\hat{n} = (n_x, n_y, \sqrt{1-n_x^2-n_y^2})$, i.e. $\vec{\lambda} = (n_x, n_y)$. Taylor expanding:

$$|\uparrow_{\hat{n}}\rangle \approx \begin{pmatrix} 1 \\ (n_x+in_y)/2 \end{pmatrix},\quad \partial_{n_x}|\uparrow_{\hat{n}}\rangle \approx \frac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix},\quad \partial_{n_y}|\uparrow_{\hat{n}}\rangle = \frac{1}{2}\begin{pmatrix} 0 \\ i \end{pmatrix}$$

using $e^{i\varphi}\sin\theta/2 \overset{\theta\ll 1}{\approx} e^{i\varphi}\frac{1}{2}\sin\theta = \frac{1}{2}(\cos\varphi + i\sin\varphi)\sin\theta = (n_x+in_y)/2$



Write $\qquad d\vec S = \hat n \, dS$

$$\vec{\tilde F}(\vec\lambda) = \nabla_{\vec\lambda} \times \vec{\tilde A}(\vec\lambda) = (\partial_{n_x} A_{n_y} - \partial_{n_y} A_{n_x})\,\hat n$$

normal to the tangent plane

with

$$\begin{cases} A_{n_x} = \underbrace{\langle \uparrow_{\hat n} |}_{(1\ (n_x - i n_y)/2)}\, \overbrace{i\partial_{n_x} | \uparrow_{\hat n}\rangle}^{\begin{pmatrix} 0 \\ \frac{i}{2} \end{pmatrix}} \approx \frac{i}{4}(n_x - i n_y) \Rightarrow \partial_{n_y} A_{n_x} = \frac{1}{4} \\ A_{n_y} = \langle \uparrow_{\hat n} | i\partial_{n_y} | \uparrow_{\hat n}\rangle \approx -\frac{1}{4}(n_x - i n_y) \Rightarrow \partial_{n_x} A_{n_y} = -\frac{1}{4} \end{cases}$$

and read off:

$$\vec{\tilde F}(\vec\lambda) \approx -\frac{1}{2}\hat n .$$

N.B. This holds anywhere on the Bloch sphere. Simply rotate the coordinate system!

$$\Rightarrow \quad \phi = \int_{\substack{S \text{ of} \\ \text{unit solid} \\ \text{angle}}} -\frac{1}{2}\hat n \cdot d\vec S = -\frac{1}{2}$$

$$\Rightarrow \quad \phi' = \int_{\substack{S:\text{ one} \\ \text{octant}}} -\frac{1}{2}\hat n \cdot d\vec S = -\frac{1}{2}\cdot\frac{1}{8}\,4\pi = -\frac{\pi}{4}$$

in agreement with our discretized calculation

HW A nice corollary: Rotate the spinor around a full great circle, say, $\hat z \to \hat x \to -\hat z \to -\hat x \to \hat z$.
The Berry phase picked up by the spinor is then

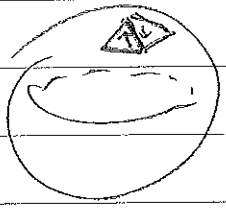
$$\phi = -\frac{1}{2}\cdot(\text{solid angle of a hemisphere}) = -\frac{1}{2}\cdot 2\pi = -\pi$$

$$|\uparrow_{\hat z}\rangle \xrightarrow[\text{one revolution}]{} e^{i\phi}|\uparrow_{\hat z}\rangle = e^{-i\pi}|\uparrow_{\hat z}\rangle = -|\uparrow_{\hat z}\rangle .$$

THE MOST IMPORTANT MINUS SIGN IN PHYSICS EXPLAINED!

From the analysis above, it follows that the total Berry flux through the unit sphere is equal to

$$\Phi = \underbrace{-\tfrac{1}{2}}_{\substack{\text{Berry flux/}\\ \text{unit solid}\\ \text{angle}}} \times 4\pi = -2\pi \qquad (\text{I}.21)$$



Assume that we partition the unit sphere into small triangles and calculate the Berry phase $\oint_\Delta \vec{A} \cdot \underbrace{d\vec{\ell}}_{\text{"}d\lambda\text{"}}$ around each triangle. The sum of these must vanish since each side of a triangle is traversed in the opposite direction for its neighbor.

$$0 \overset{?}{=} -2\pi \;.$$

Let's call the Berry flux Φ_S $\left(= \oint_S \vec{F} \cdot d\vec{S}\right)$ ← integral over the closed surface S

— " — Berry phase Φ_Γ $\left(= \oint \vec{A} \cdot d\vec{\ell}\right)$ ↑ path Γ

Now, recall that Φ_Γ is defined only mod 2π (depending on choice of gauge!)
If Φ_Γ is to be equal to Φ_S, Φ_S must therefore take (some unique!) value $2\pi C$, where C is an integer

⇓

$$\oint_S \vec{F} \cdot d\vec{S} = 2\pi C \qquad (\text{I}.22)$$

CHERN THEOREM

CHERN NUMBER

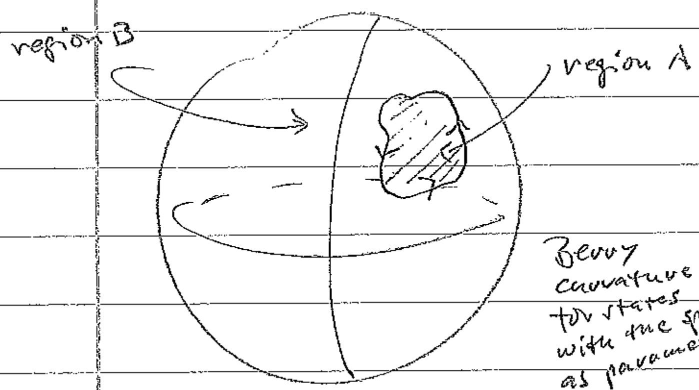
$\Phi_\Gamma = 0, \pm 2\pi, \pm 4\pi \ldots$ depending on choice of gauge. Which gauge is the "correct" one, ensuring that $\Phi_\Gamma = \Phi_S$

ALWAYS "CORRECT"!

HW

Answer: The gauge that is smooth and continuous everywhere in S, and on Γ!

Let's attempt a continuum proof of the Chern theorem, using again a sphere as illustration. Divide the sphere in two regions, A and B.



$$\oint_A \vec{F}\cdot d\vec{S} = \phi_p \bmod 2\pi \quad (a)$$

Berry curvature for states with the sphere as parameter space

$\uparrow$ calculated as the Berry phase around the boundary between A and B

$$-\oint_B \vec{F}\cdot d\vec{S} = \phi_p \bmod 2\pi \quad (b)$$

– sign because the boundary of B is traversed in the opposite direction

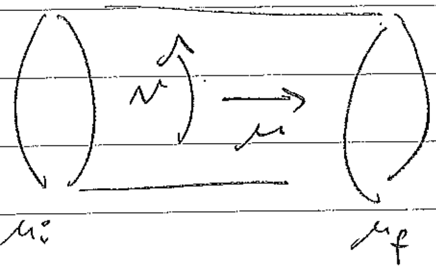
Subtracting the two equations (a) and (b) :

$$\underbrace{\oint_A \vec{F}\cdot d\vec{S} - \left(-\oint_B \vec{F}\cdot d\vec{S}\right) = \oint_{A\cup B = S} \vec{F}\cdot d\vec{S} = 0 \bmod 2\pi}_{\text{CHERN THEOREM}}$$

(I.23)

DISCUSSION : A nonzero Chern number presents a topological obstruction to construct a globally smooth gauge. (Cf. discussion on the previous page!)

To develop some intuition for what the Chern number measures, let's look at the Berry flux on a cylinder, with parameters ν and μ:



Let $\nu \in [0,1]$ with $\nu=0$ and $\nu=1$ identified.

Assume a periodic gauge in the ν-direction:

$|u_{\mu,\nu=0}\rangle = |u_{\mu,\nu=1}\rangle$. Then the Berry flux on the cylinder can be written

$$\Phi^{(\mu\nu)} = \int_{\mu_i}^{\mu_f} d\mu \int_0^1 d\nu \, (\partial_\mu A_\nu - \cancel{\partial_\nu A_\mu})$$

$$\left\{ \int_0^1 d\nu \, \partial_\nu A_\mu = A_\mu \Big|_0^1 = 0 \text{ since } A_\mu = \langle u_{\mu,\nu} | i\partial_\mu | u_{\mu,\nu}\rangle \right\}$$

$$\int_{S} \vec{F}(\vec{\lambda}) \cdot d\vec{S} = \int_S (\partial_\mu A_\nu - \partial_\nu A_\mu) \underbrace{\hat{n}\cdot\hat{n}}_{=1} \underbrace{dS}_{d\mu\, d\nu}, \quad \vec{\lambda} = (\mu,\nu)$$

S = cylinder ~~surface~~ $\hat{n}$

Now, the Berry phase $\phi^{(\nu)}$ in the ν-direction is given by

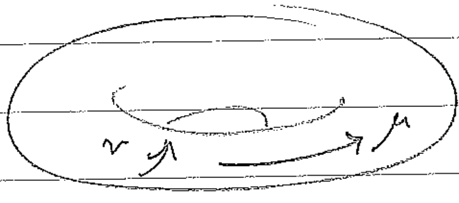
$$\phi^{(\nu)} = \int_0^1 A_\nu \, d\nu$$

and it follows that

$$\Phi^{(\mu\nu)} = \int_{\mu_i}^{\mu_f} (\partial_\mu \phi^{(\nu)}) \, d\mu = \phi^{(\nu)}(\mu_f) - \phi^{(\nu)}(\mu_i)$$

~~If we follow the evolution of $\phi^{(\nu)}$ (no 2π jumps!),~~

In words: the Berry flux on the cylinder is given by the change of the Berry phase $\phi^{(\nu)}$ during the evolution.



Now turn to a 2-torus,
where also $\mu_i = 0$ and $\mu_f = 1$
are identified. The Berry phase $\phi^{(\nu)}$ at the two end points
must match mod 2π, i.e. $\phi^{(\nu)}$ must have evolved
by $2\pi m$ at the end of the cycle on μ

$$\Downarrow$$

$$\phi^{(\mu\nu)} = \phi^{(\nu)}(\mu=1) - \phi^{(\nu)}(\mu=0) = 2\pi m$$

$$= \oint \tilde{F}^{(\mu\nu)} d\mu d\nu = 2\pi C^{(\mu\nu)}_{\text{"First"}}$$

↑ Chern number (since in 2D)

$$\overbrace{\;}^{\text{wow!}} \Rightarrow \; m = C^{(\mu\nu)}$$

The Chern number $\overset{\text{on a 2-torus}}{=}$ winding number of the Berry phase along ν as we evolve around a cycle in μ.

$\sim$

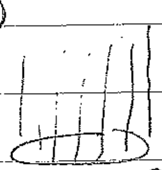
"FIRST": B is 2D ✓ "SECOND": ~~B is 4D~~

Brief discussion of Chern classes and fiber bundles
(complex vector bundles)

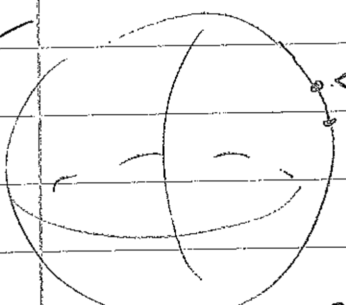
$$E = B \times F$$

↑ base manifold ↑ "fiber"

EX 1



EX 2



Associate a complex vector space F (e.g. $F = \mathbb{C}^2$) to each point of B.

$B = S^2$ parameters (θ, φ)

Next:
Adiabatic dynamics!

How does the Berry phase relate to the time evolution of a system as governed by the Schrödinger equation?

Consider a Hamiltonian $H(\lambda)$ with λ being a "slow" function of time t. Roughly speaking, "slowness" (or ADIABATIC TIME EVOLUTION) is guaranteed if the rate of variation of λ with time is slow compared to $\Delta E/\hbar$ where ΔE is a typical spacing between energy levels.
For a given λ, the (instantaneous) eigenstates of H are

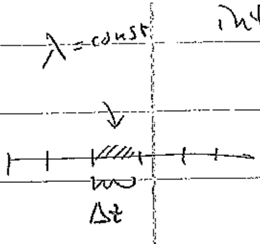
$$H(\lambda)|n(\lambda)\rangle = E_n(\lambda)\,|n(\lambda)\rangle \qquad (\text{I}.23)$$

If λ did not vary with t, the state would evolve as

$\psi(t) \equiv n(t)$ $\qquad n = n(t=0)$

$$|\psi(t)\rangle = e^{-iE_n t/\hbar}\,|n\rangle \qquad (\text{I}.24)$$

In contrast, if λ changes with time, but so slowly that we can approximate it as constant in each small time interval Δt, the time evolution would be governed by



$$\sim e^{-iE_n(\lambda_1)\Delta t/\hbar}\; e^{-iE_n(\lambda_2)\Delta t/\hbar} \cdots$$

$$= \prod_{\Delta t} e^{-iE_n(\lambda(t))\Delta t/\hbar} = \prod_{\Delta t} e^{-iE_n(t)\Delta t/\hbar}$$

$$= e^{-i\sum_{\Delta t} E_n(t)\Delta t/\hbar} \equiv e^{-i\gamma(t)} \qquad \text{ordinary dynamical phase } (\text{I}.25)$$

$$\gamma(t) = \frac{1}{\hbar}\sum_{\Delta t} E_n(t) \xrightarrow{\text{continuum limit}} \frac{1}{\hbar}\int \underbrace{E_n(t')}_{E_n(\lambda(t'))}\,dt' \,. \qquad (\text{I}.26)$$

This leads to the Ansatz

$$|\psi(t)\rangle = c(t)\, e^{-i\gamma(t)}\, |u(t)\rangle \qquad (\mathrm{I}.27)$$

to allow for a possible extra phase beyond $e^{-i\gamma(t)}$

recall: $|u(\lambda(t))\rangle$ = eigenstate of the time-independent problem evaluated at $\lambda = \lambda(t)$

Plug this Ansatz into the time-dependent Schrödinger eq.

$$\left(i\hbar\partial_t - H(t)\right)|\psi(t)\rangle = 0 \qquad (\mathrm{I}.28)$$

to find that

$$\dot{c}(t)\,|u(t)\rangle + c(t)\,\partial_t|u(t)\rangle = 0 \qquad (\mathrm{I}.29)$$

Argument:

From (I.27), (I.28), $i\hbar\left(\dot{c}(t)e^{-i\gamma(t)}|u(t)\rangle + c(t)\cancel{(-i\dot{\gamma}(t))e^{-i\gamma(t)}}|u(t)\rangle\right.$ $\left. + c(t)e^{-i\gamma(t)}\partial_t|u(t)\rangle\right) - c(t)\cancel{e^{-i\gamma(t)}E_n(t)}|u(t)\rangle = 0$ using that $\dot{\gamma}(t) = E_n(t)/\hbar$ from (I.26)

Multiplying (I.29) from the left by $\langle u(t)|$ it follows that

$$\dot{c}(t) = i\,c(t)\,A_n(t) \qquad (\mathrm{I}.30)$$

where $A_n(t) = \langle u(t)|\,i\partial_t\,|u(t)\rangle$ is a Berry connection "in time"*. The solution of (I.30) is given by $c(t) = e^{i\phi(t)}$ with

$$\phi(t) = \int_0^t A_n(t')\,dt' \qquad (\mathrm{I}.31)$$

open-path Berry phase

recall
* $A_n(t) = A_n(\lambda(t))$

(I.18

We can reexpress this open-path Berry phase in terms of the time-dependent parameter λ instead of t, using that $\partial_t |u(t)\rangle = \dot{\lambda}\, \partial_\lambda |u(\lambda)\rangle$. As a result $A_n(t) = \dot{\lambda}\, A_n(\lambda)$ where

$$A_n(\lambda) = \langle u(\lambda) | i\partial_\lambda | u(\lambda)\rangle \qquad (\text{I}.32)$$

is the "usual" Berry connection in parameter space. It follows that

$$\phi(t) \overset{(\text{I}.31)}{=} \int_0^t A_n(t')\,dt' = \int_{\lambda(0)}^{\lambda(t)} A_n(\lambda) \frac{d\lambda}{dt'}\,dt'$$

$$= \int_{\lambda(0)}^{\lambda(t)} A_n(\lambda)\, d\lambda \qquad (\text{I}.33)$$

Note that $\phi(t)$ only depends on the path, not the rate of change (as long as it is adiabatic)

$\Rightarrow$ "GEOMETRIC PHASE"

$\Downarrow$

$$|\Psi(t)\rangle = e^{i\phi(\lambda(t))}\, e^{-i\gamma(t)}\, |u(t)\rangle \qquad (\text{I}.34)$$

Discussion of influence of higher-order terms in the Ansatz (I.27).

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Let's leave the problem of adiabatic transport for a while (what will be!) and now focus on the main theme in this first part of the course: Berry phases, connections, fluxes, and curvatures for states defined on the Brillouin zone (BZ) for electrons in a BAND INSULATOR. This belongs to the subject of TOPOLOGICAL BAND THEORY.