

## Lect 29      Berry phase

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Let us consider a Hamiltonian depending on an external parameter  $H(\vec{R})$ , and  $\vec{R}$  is a slow variable of time :  $\vec{R}(t)$ .

For each  $\vec{R}$ , we define its eigenstate  $\psi_n(\vec{R})$ .

$$H(\vec{R}) \psi_n(\vec{R}) = E_n(\vec{R}) \psi_n(\vec{R})$$

Now let us consider the time dependent problem

$$i\hbar \frac{\partial}{\partial t} \psi(t) = H(\vec{R}(t)) \psi(t), \text{ and } \psi(t=0) = \psi_n(\vec{R}(t=0))$$

Suppose  $R(t)$  varies sufficiently slow, so the adiabatic theory can be applied.

apply. we write  $i \int dt' F_{\perp}(R) + i \gamma_n(t)$

$$\psi(t) = e^{-i \int_0^t E_n(R) dt} e^{+i \gamma_n(t)} \psi_n(R(t))$$

dynamic phase      Bern

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \psi(t) = \left[ E_n(\vec{R}(t)) \checkmark + i\hbar \frac{\partial}{\partial t} \sigma_n \right] \psi(t)$$

$$+ e^{-i \int_0^t dt' \frac{E_n(\vec{R})}{\hbar}} e^{-i \sigma_n(t)} i\hbar \frac{\partial}{\partial t} \psi_n(\vec{R}(t))$$

$$= E_n(\vec{R}(t)) \psi(t)$$

$$\Rightarrow +\hbar \frac{\partial}{\partial t} \gamma_n(t) \psi_n(\vec{R}(t)) = -i\hbar \frac{\partial}{\partial t} \psi_n(\vec{R}(t))$$

$$\frac{\partial}{\partial t} \tilde{\gamma}_n(t) = -i \langle \psi_n(\vec{R}(t)) | \frac{\partial}{\partial t} | \psi_n(\vec{R}(t)) \rangle$$

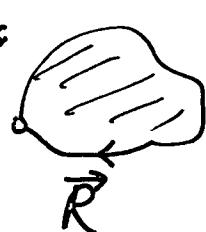
Change  $\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial \vec{R}} \cdot \frac{\partial \vec{R}}{\partial t} \Rightarrow$

$$\frac{\partial}{\partial \vec{R}} \tilde{\gamma}_n(\vec{R}) = -i \langle \psi_n(\vec{R}) | \frac{\partial}{\partial \vec{R}} | \psi_n(\vec{R}) \rangle = \vec{A}(\vec{R})$$

↑ Berry connection

After a closed path in the parameter space,  $\vec{R}$  comes back to the initial value. But the state vector  $\psi_n$  gains

$$\tilde{\gamma}_n = \oint d\vec{R} \cdot \vec{A}(\vec{R})$$



$$= \iint_S d\vec{S} \cdot \vec{B}(\vec{R})$$

where  $\vec{B}(\vec{R}) = \nabla_{\vec{R}} \times \vec{A}(\vec{R})$  ← Berry curvature.

→ Gauge transformation

Gauge transformation: the instant eigenstate  $\psi_n(R)$  is only well-defined up to a phase factor. If

$$\psi_n(R) \rightarrow \psi'_n(R) = e^{-i\alpha_n(R)} \psi_n(R)$$

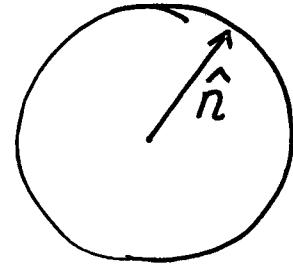
$$\vec{A}(R) \rightarrow \vec{A}'(R) = i \langle \psi'_n(R) | \frac{\partial}{\partial R} | \psi'_n(R) \rangle = i \langle \psi_n | \frac{\partial}{\partial R} | \psi_n \rangle$$

$$\Rightarrow \nabla_{\vec{R}} \times \vec{A}(R) = \nabla_{\vec{R}} \times \vec{A}'(R) + \nabla_R \alpha_n(R)$$

Example: two energy-level system. Spin- $1/2$  particle in a magnetic field  $\vec{B} = B \hat{n}$ . As  $\hat{n}$  varies, we calculate Berry phase.

Let us first solve the eigenstates of  $H = -\vec{B} \cdot \vec{\sigma}$ .

$$H = -B \hat{n} \cdot \vec{\sigma}.$$



Introduce projection operators

$$P_{\pm} = \frac{1}{2}(I + \hat{n} \cdot \vec{\sigma}) \quad \text{check} \quad P_{\pm}^2 = \frac{1}{4}(I + I \pm 2\hat{n} \cdot \vec{\sigma}) = P_{\pm}$$

$$P_+ = \frac{1}{2} \begin{pmatrix} 1+n_3 & n_1 - in_2 \\ n_1 + in_2 & 1-n_3 \end{pmatrix}, \quad P_- = \frac{1}{2} \begin{pmatrix} 1-n_3 & n_1 + in_2 \\ n_1 - in_2 & 1+n_3 \end{pmatrix}.$$

$$H P_{\pm} = \mp B P_{\pm}, \quad P_+ + P_- = 1. \quad P_+ \circ P_- = P_- \circ P_+ = 0.$$

$\Rightarrow$  for any state vector  $| \psi \rangle = P_+ | \psi \rangle + P_- | \psi \rangle$

$$\Rightarrow H(P_+ | \psi \rangle) = -P_+ | \psi \rangle, \quad H(P_- | \psi \rangle) = +P_- | \psi \rangle.$$

i.e.  $P_+$  and  $P_-$  decompose the Hilbert space into two eigen states.

say let me choose  $| \psi \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ , we have the low energy

eigenstate

$$| \psi_{+}^{(1)}(\hat{n}) \rangle = \frac{1}{N} P_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{N} \begin{pmatrix} 1+n_3 \\ n_1 + in_2 \end{pmatrix} = \frac{1}{\sqrt{2(1+n_3)}} \begin{pmatrix} 1+n_3 \\ n_1 + in_2 \end{pmatrix}$$

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the high energy state

$$|\psi_H^{(1)}(\hat{n})\rangle = \frac{1}{N} P_-\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{N} \begin{pmatrix} 1-n_3 \\ n_1-in_2 \end{pmatrix} = \frac{1}{\sqrt{2(1-n_3)}} \begin{pmatrix} 1-n_3 \\ n_1-in_2 \end{pmatrix}$$

or we can use that state  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  for projection

$$|\psi_L^{(2)}(\hat{n})\rangle = \frac{1}{N} \begin{pmatrix} n_1-in_2 \\ 1-n_3 \end{pmatrix} = \frac{1}{\sqrt{2(1-n_3)}} \begin{pmatrix} n_1-in_2 \\ 1-n_3 \end{pmatrix}$$

$$|\psi_H^{(2)}(\hat{n})\rangle = \frac{1}{N} \begin{pmatrix} n_1+in_2 \\ 1+n_3 \end{pmatrix} = \frac{1}{\sqrt{2(1+n_3)}} \begin{pmatrix} n_1+in_2 \\ 1+n_3 \end{pmatrix}$$

Next we calculate Berry connection / Berry curvature.

For low energy level and gauge 1  $\Rightarrow$

$$\frac{d}{dt} |\psi_i^{(1)}(\hat{n}(t))\rangle = \frac{1}{\sqrt{2(1+n_3)}} \begin{pmatrix} \dot{n}_3 \\ \dot{n}_1+in_2 \end{pmatrix} + \frac{-\dot{n}_3}{2\sqrt{2(1+n_3)^{3/2}}} \begin{pmatrix} 1+n_3 \\ n_1+in_2 \end{pmatrix}$$

$$\begin{aligned} \langle \psi_L^{(1)}(\hat{n}(t)) | \frac{d}{dt} |\psi_L^{(1)}(\hat{n}(t))\rangle &= \frac{1}{2(1+n_3)} \left[ (1+n_3) \dot{n}_3 + (n_1-in_2)(\dot{n}_1+in_2) \right] \\ &\quad - \frac{1}{4(1+n_3)^2} \left[ (1+n_3)^2 \dot{n}_3 + (n_1^2+n_2^2) \dot{n}_3 \right] \end{aligned}$$

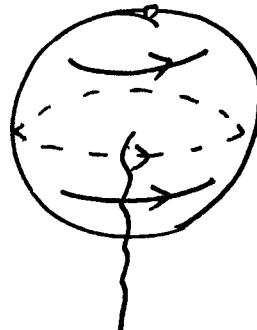
$$\begin{aligned} &= \frac{1}{2(1+n_3)} \left[ \dot{n}_3 + n_3 \dot{n}_3 + n_1 \dot{n}_1 + n_2 \dot{n}_2 + i(n_1 \dot{n}_2 - n_2 \dot{n}_1) - \frac{1}{2} [(1+n_3) \dot{n}_3 + (1-n_3) \dot{n}_3] \right] \end{aligned}$$

$$= \frac{i}{2(1+n_3)} (n_1 \dot{n}_2 - n_2 \dot{n}_1)$$

$$\gamma_{i,L} = -i \int dt A(t) = -i \int d\vec{n} \langle \psi_L^{(i)} | \nabla_n | \psi_L^{(i)} \rangle$$

$$= \int dN_\alpha A_\alpha(\hat{n})$$

where  $A_\alpha dN_\alpha = \frac{1}{2(1+n_3)} (n_1 dn_2 - n_2 dn_1)$



we can choose  $A_1 = \frac{-n_2}{2(1+n_3)}$ ,  $A_2 = \frac{n_1}{2(1+n_3)}$ ,  $A_3 = 0$

$$\Rightarrow A_1 = \frac{-\sin\theta \sin\varphi}{2(1+\cos\theta)} = -\frac{\sin\varphi}{2} \operatorname{tg}\frac{\theta}{2} \quad \left. \right\} \Rightarrow \vec{A} = \frac{1}{2} \operatorname{tg}\frac{\theta}{2} \hat{e}_\varphi$$

$$(n)$$

$$A_2 = +\frac{\cos\varphi}{2} \operatorname{tg}\frac{\theta}{2}, \quad A_3 = 0$$

$\vec{A}$  has a singular point at south pole  $n_3 = -1$ .

using the formula

$$\nabla \times \vec{A} = \frac{1}{r \sin\theta} \left( \frac{\partial}{\partial \theta} (\sin\theta A_\varphi) - \frac{\partial A_\theta}{\partial \varphi} \right) \hat{e}_r$$

$$+ \left( \frac{1}{r \sin\theta} \frac{\partial A_r}{\partial \varphi} - \frac{1}{r} \frac{\partial}{\partial r} (r A_\varphi) \right) \hat{e}_\theta$$

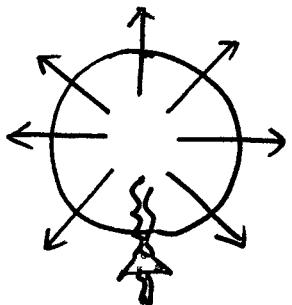
$$+ \left[ \frac{1}{r} \frac{\partial}{\partial r} (r A_\theta) - \frac{1}{r} \frac{\partial A_r}{\partial \theta} \right] \hat{e}_\varphi$$

Plug in  $\Rightarrow \nabla \times \vec{A} = \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left[ \frac{1}{2} 2 \sin^2 \frac{\theta}{2} \right] \hat{e}_r = \frac{1}{2} \hat{e}_r$

Magnetic Monopole field !!!

How can a curl describe a monopole field?  $\nabla \cdot (\nabla \times \vec{A}) = 0$   
 $\nabla \cdot (\hat{\mathbf{e}}_r) \neq 0$ ?

Singularity: Dirac String / Dirac monopole



$\vec{A}$  is not well-defined over the entire sphere

Let us choose a small path around south pole

$$\theta = \pi \bar{\theta} \theta^+, \quad \varphi: 0 \rightarrow 2\pi$$

$$\oint A^a d\omega_a = -2\pi \sin \theta \left. \frac{1}{2} \operatorname{tg} \frac{\theta}{2} \right|_{\theta \rightarrow \pi} \\ = -\pi \left. 2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cdot \sin \frac{\theta}{2} / \cos \frac{\theta}{2} \right|_{\theta \rightarrow \pi} = -2\pi$$

$$\Rightarrow \nabla \times \vec{A} = \frac{1}{2} (1 - 4\pi \delta(\vec{r} = \text{south pole})) \hat{\mathbf{e}}_r$$

↗ Dirac string

however, the Dirac string should not

be physical, because we have rotational symmetry.  $\vec{B}$  should be uniform over the entire sphere. This is the artifact that, we insist to use vector potential to describe a monopole field.

Let us recalculate the Berry connection and Berry curvature,

but use a different gauge  $|\psi_L^{(z)}\rangle = \frac{1}{\sqrt{2(1-n_3)}} \begin{pmatrix} n_1 - in_2 \\ 1 - n_3 \end{pmatrix}$

$$\frac{d}{dt} |\psi_L^{(z)}(\hat{n}(t))\rangle = \frac{1}{\sqrt{2(1-n_3)}} \begin{pmatrix} \dot{n}_1 - i\dot{n}_2 \\ -\dot{n}_3 \end{pmatrix} + \frac{\dot{n}_3}{2\sqrt{(1-n_3)^{3/2}}} \begin{pmatrix} n_1 - in_2 \\ 1 - n_3 \end{pmatrix}$$

Similarly we will get

$$\begin{aligned}\langle \psi_L^{(2)} | \frac{d}{dt} | \psi_L^{(2)} \rangle &= \frac{1}{2(1-n_3)} [(n_1 + in_2)(\dot{n}_1 - in_2) + (1-n_3)(-\dot{n}_3)] \\ &\quad + \frac{1}{4(1-n_3)^2} [(n_1^2 + n_2^2)\dot{n}_3 + (1-n_3)^2\ddot{n}_3] \\ &= \frac{-i}{2(1-n_3)} [n_1\dot{n}_2 - n_2\dot{n}_1]\end{aligned}$$

$$\tilde{A}_\alpha dn_\alpha = \frac{-1}{2(1-n_3)} (n_1 dn_2 - n_2 dn_1) \Rightarrow \tilde{A} = -\frac{1}{2} \operatorname{ctg} \frac{\theta}{2} \hat{e}_\varphi$$

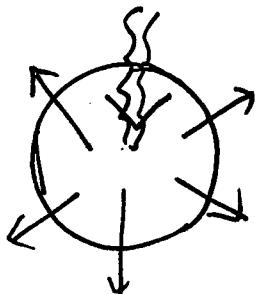
$$\tilde{A}_1 = \frac{n_2}{2(1-n_3)} = \frac{\sin\theta \sin\varphi}{2(1-\cos\theta)} = \frac{\sin\varphi}{2} \operatorname{ctg} \frac{\theta}{2} \quad \uparrow$$

$$\tilde{A}_2 = \frac{-n_1}{2(1-n_3)} = \frac{-\sin\theta \cos\varphi}{2(1-\cos\theta)} = -\frac{\cos\varphi}{2} \operatorname{ctg} \frac{\theta}{2}$$

$$\nabla \times \tilde{A} = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left( -\frac{1}{2} 2 \cos \frac{\theta}{2} \right) \hat{e}_r = \frac{1}{2} \hat{e}_r$$

the singular point is at the north pole.

Let us choose a small loop at  $\theta = 0^+$



$$\oint \tilde{A}_\alpha dn_\alpha = \sin\theta \left(-\frac{1}{2}\right) \operatorname{ctg} \frac{\theta}{2} \cdot 2\pi \Big|_{\theta \rightarrow 0^+} = -2\pi$$

$$\nabla \times \tilde{A} = \frac{1}{2} [1 - 2\pi \delta(\hat{n} = \text{north pole})] \hat{e}_r$$

Dirac monopole defines a topologically non-trivial  $U(1)$  fiber bundle over the two-sphere  $S^2$ . We are not able define well-defined  $\vec{A}$  over the entire sphere. If you insist to use a single definition of  $\vec{A}$ , you suffer from the unphysical Dirac string. (An analogy in differential geometry is that, you cannot define a non-singular coordinate over a sphere. This is a result of the intrinsic curvature).

The best job we can do: cut the sphere into two hemisphere.

$A_\alpha$  is well-defined in northern hemisphere } ← Locally  
 $\tilde{A}$  is well-defined in the south hemisphere } but not globally

They overlap at the equator, in which

$$\tilde{A}_\alpha = A_\alpha - i \omega^{-1} \partial_\alpha \omega \quad \omega = e^{-i\varphi} \leftarrow \text{gauge transform}$$

At equator  $|\psi_L^{(0)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ n_1 + in_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\varphi} \end{pmatrix} = e^{i\varphi} |\psi_u^{(1)}\rangle$

$$|\psi_L^{(\omega)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} n_1 - in_2 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi} \\ 1 \end{pmatrix}$$

$\omega$  is also the group space of  $U(1)$

This maps the equator  $S^1 \rightarrow U(1)$  group space.

We can define the winding number  $C_1$ ,

$$2\pi C_1 = i \oint_{S^1} \omega^{-1} \partial_\alpha \omega d\eta_\alpha$$

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$$2\pi C_1 = \oint_{S_1} A^a d\eta_a - \oint_{S_1} \tilde{A}^a d\eta_a$$

$$= \iint_{\text{north}} d\vec{s} \cdot \vec{B} + \iint_{\text{south}} d\vec{s} \cdot \vec{B} = \oint d\vec{s} \cdot \vec{B}$$

Winding number

$C_1$  has to be integer :  $i \oint_{S_1} \omega^{-1} \partial_\varphi \omega d\eta_a$  generally speaking

$\omega = e^{i\delta(\varphi)}$

$\xrightarrow{\text{U}(1)}$

$= i \int_0^{2\pi} d\varphi e^{i\delta(\varphi)} \partial_\varphi e^{-i\delta(\varphi)}$

$S_1$  equation  $\boxed{\Pi_1(U(1)) = \mathbb{Z}}$

$= \int_0^{2\pi} d\varphi \partial_\varphi \delta(\varphi) = \oint d\delta = \uparrow \text{angle is multiple valued.} Z\pi C_1$

$$\Rightarrow \oint d\vec{s} \cdot \vec{B} = 2\pi C_1$$

the first Chern number!

For the Low energy level  $C_1 = 1$ .

Similarly, we can repeat the above calculation, and arrive at the Berry connection / curvature for the high energy level, which is also a monopole with opposite charge -1.

$$\oint \vec{B}_H \cdot d\vec{s} = \oint_{S_1} A_H^a d\eta_a - \oint_{S_1} \tilde{A}_H^a d\eta_a = -2\pi$$

## § Sum-rule of Berry curvature

$$F_{\mu\nu}^n(\vec{R}) = \frac{\partial}{\partial R_\mu} A_\nu^n(R) - \frac{\partial}{\partial R_\nu} A_\mu^n(R) = i \left\{ \left\langle \frac{\partial}{\partial R_\mu} \psi^n | \frac{\partial}{\partial R_\nu} \psi^n \right\rangle - \left\langle \frac{\partial}{\partial R_\nu} \psi^n | \frac{\partial}{\partial R_\mu} \psi^n \right\rangle \right\}$$

if we sum over all the energy levels  $n$ , all the Berry curvatures add

$$\sum_n F_{\mu\nu}^n(\vec{R}) = 0$$

to zero.

**Proof:** Let us denote the basis  $\psi_n(\vec{R})$   $n=1, 2, \dots$  at  $\vec{R}$ . And we expand eigenstates at  $\psi_n(\vec{R} + \Delta\vec{R})$  in terms of  $\psi_n(\vec{R})$ . Assume  $H(\vec{R} + \Delta\vec{R}) = H(\vec{R}) + \nabla_{\vec{R}}H \cdot \Delta\vec{R}$ . From perturbation theory

$$|\psi_n(R + \Delta R)\rangle = |\psi_n(R)\rangle + \sum'_m \frac{|\psi_m(\vec{R})\rangle \langle \psi_m(\vec{R})| \nabla_{\vec{R}}H | \psi_n(\vec{R})\rangle \cdot \Delta\vec{R}}{E_n - E_m}$$

$$\vec{\nabla}_{\vec{R}} |\psi_n(\vec{R})\rangle = \sum'_m \frac{|\psi_m(\vec{R})\rangle \langle \psi_m(\vec{R})| \nabla_{\vec{R}}H | \psi_n(\vec{R})\rangle}{E_n - E_m}$$

$$\sum_n \left\{ \langle \nabla_{R_\mu} \psi_n | \nabla_{R_\nu} \psi_n \rangle - \langle \nabla_{R_\nu} \psi_n | \nabla_{R_\mu} \psi_n \rangle \right\} = \sum'_{m,n} \frac{1}{(E_n - E_m)^2}$$

$$\left\{ \langle \psi_n(R) | \nabla_{R_\mu} H | \psi_m(R) \rangle \langle \psi_m(R) | \nabla_{R_\nu} H | \psi_n(R) \rangle - (\mu \leftrightarrow \nu) \right\} = 0.$$

under exchange  $m \leftrightarrow n$ , the above equation is odd

$\Rightarrow$  sum to zero.