

Lect 29 Berry phase

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 apply. we write

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

dynamic phase ← Berry phase

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \psi(t) = \left[E_n(\vec{R}(t)) + \hbar \frac{\partial}{\partial t} \gamma_n \right] \psi(t) + e^{-i \int_0^t dt' \frac{E_n(\vec{R})}{\hbar}} e^{-i \gamma_n(t)} i\hbar \frac{\partial}{\partial t} \psi_n(\vec{R}(t)) = E_n(\vec{R}(t)) \psi(t)$$

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

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

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

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

↑ Berry connection

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

$$\gamma_n = \oint d\vec{R} \cdot \vec{A}(\vec{R})$$



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

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

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

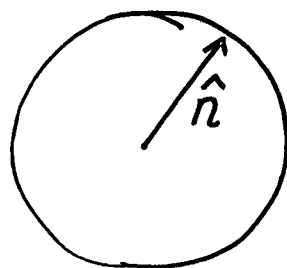
$$\psi_n(\vec{R}) \rightarrow \psi'_n(\vec{R}) = e^{-i\alpha_n(\vec{R})} \psi_n(\vec{R})$$

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

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

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

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

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

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

\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 eigenstates.

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

eigenstate

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

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

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

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

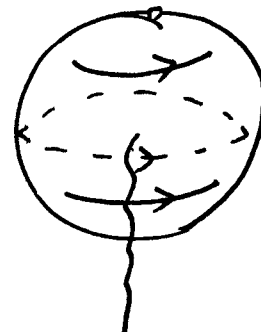
$$= \frac{1}{2(1+n_3)} \left[\dot{n}_3 + n_3 \dot{n}_3 + n_1 \dot{n}_1 + n_2 \dot{n}_2 + i(n_1 \dot{n}_2 - n_2 \dot{n}_1) - \frac{1}{2} \left[(1+n_3) \dot{n}_3 + (1-n_3) \dot{n}_3 \right] \right]$$

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

$$\gamma_{r_L} = -i \int dt A(t) = -i \int d\vec{n} \langle \psi_L^{(0)} | \nabla_n | \psi_L^{(0)} \rangle$$

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

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



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

$$\Rightarrow \left. \begin{aligned} A_1 &= \frac{-\sin\theta \sin\varphi}{2(1+\cos\theta)} = -\frac{\sin\varphi}{2} \operatorname{tg} \frac{\theta}{2} \\ A_2 &= +\frac{\cos\varphi}{2} \operatorname{tg} \frac{\theta}{2}, \quad A_3 = 0 \end{aligned} \right\} \Rightarrow \vec{A} = \frac{1}{2} \operatorname{tg} \frac{\theta}{2} \hat{e}_\varphi(\hat{n})$$

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

using the formula

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

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

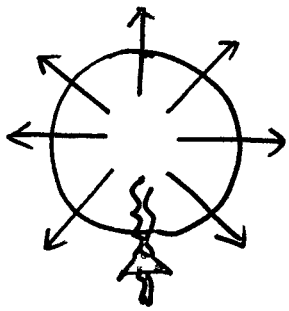
$$+ \left[\frac{1}{r} \frac{\partial}{\partial r} (r A_\theta) - \frac{1}{r} \frac{\partial A_r}{\partial\theta} \right] \hat{e}_\varphi$$

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? $\nabla \cdot (\nabla \times A) = 0$
 $\nabla \cdot (\hat{e}_r) \neq 0$?

Singularity: Dirac string / Dirac monopole



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

Let us choose a small path around south pole

$$\theta = \pi - \epsilon, \varphi: 0 \rightarrow 2\pi$$

$$\oint A_a dn_a = -2\pi \sin \theta \frac{1}{2} \tan \frac{\theta}{2} \Big|_{\theta \rightarrow \pi}$$
$$= -\pi \cdot 2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cdot \frac{\sin \frac{\theta}{2}}{\cos \frac{\theta}{2}} = -2\pi$$

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

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

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

Similarly we will get

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

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

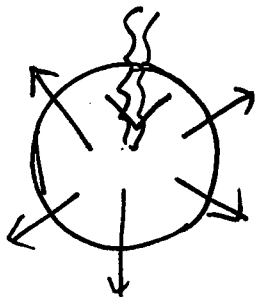
$$\tilde{A}_1 = \frac{n_2}{2(1-n_3)} = \frac{\sin\theta \sin\varphi}{2(1-\cos\theta)} = \frac{\sin\varphi}{2} \operatorname{ctg} \frac{\theta}{2}$$

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

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

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 to 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 hemispheres.

A_α is well-defined in northern hemisphere } ← Locally
 \tilde{A} is well-defined in the southern 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 $|\psi_L^{(u)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ n_1 + im_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\varphi} \end{pmatrix} = e^{-i\varphi} |\psi_L^{(u)}\rangle$

$$|\psi_L^{(s)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} n_1 - im_2 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi} \\ 1 \end{pmatrix}$$

ω 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

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

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

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

Winding number

C_1 has to be integer: $i \oint_{S_1} \omega^{-1} \partial_\alpha \omega dn_\alpha$

generally speaking

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



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

$$= \int_0^{2\pi} d\varphi \partial_\varphi \delta(\varphi) = \oint d\delta = 2\pi C_1$$

↑ angle is multiple valued.

S_1 equation

$$\pi_1(U(1)) = \mathbb{Z}$$

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

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.

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

§ Sum-rule of Berry curvature

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

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

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

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 $H(\vec{R} + \Delta\vec{R}) = H(\vec{R}) + \nabla_R H \cdot \Delta\vec{R}$. From perturbation theory

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

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

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

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

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

\Rightarrow sum to zero.