Lect 10 Berry phase

Let us consider a Hamiltnian 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 eigen state $\psi_n(\vec{R})$.

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

Now let us consider the time dependent problem

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

Suppose $R(t)$ varies sufficiently slow, so the adiabatic theory can apply. We write

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

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

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

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

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

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

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

↑ Berry connetion

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

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

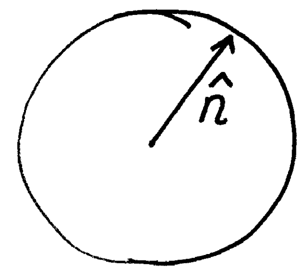
$$\psi_n(R) \rightarrow \psi_n'(R) = e^{-i\alpha_n(R)}\psi_n(R)$$

$$\vec{A}(\vec{R}) \rightarrow \vec{A}'(\vec{R}) = i\langle \psi_n'(R) | \frac{\partial}{\partial \vec{R}} | \psi_n'(R)\rangle = i\langle \psi_n | \frac{\partial}{\partial R} | \psi_n\rangle + \nabla_R\,\alpha_n(R)$$

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

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

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

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

$$\boxed{H P_\pm = \mp P_\pm H, \qquad P_+ + P_- = 1. \qquad P_+ \cdot P_- = P_- P_+ = 0.}$$

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

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

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

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

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 $\Rightarrow$

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

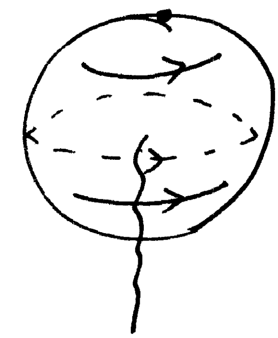
$$\langle \psi_L^{(1)}(\hat{n}(t))|\frac{d}{dt}|\psi_L^{(1)}(\hat{n}(t))\rangle = \frac{1}{2(1+n_3)}\Big[(1+n_3)\dot{n}_3 + (n_1 - in_2)(\dot{n}_1 + i\dot{n}_2)\Big]$$
$$- \frac{1}{4(1+n_3)^2}\Big[(1+n_3)^2\dot{n}_3 + (n_1^2 + n_2^2)\dot{n}_3\Big]$$

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

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

$$\gamma_L = -i\int dt\ A(t) = -i\int d\vec{n}\ \langle \psi_L^{(1)} | \nabla_n | \psi_L^{(1)} \rangle$$

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



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

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

$$\Rightarrow\ A_1 = \frac{-\sin\theta\sin\varphi}{2(1+\cos\theta)} = -\frac{\sin\varphi}{2}\, tg\frac{\theta}{2}$$

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

$$\Bigg\} \Rightarrow\ \vec{A}(\hat{n}) = \frac{1}{2} tg\frac{\theta}{2}\ \hat{e}_\varphi$$

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

using the formula

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

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

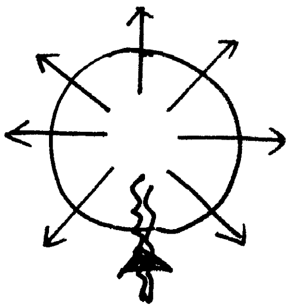
$$+\left[\frac{1}{r}\frac{\partial}{\partial r}(rA_\theta) - \frac{1}{r}\frac{\partial A_r}{\partial\theta}\right]\hat{e}_\varphi$$

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 Monople field !!!

How can a curl describe a monople 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

$\theta = \pi - 0^+,\quad \varphi: 0\to 2\pi$

$$\oint A^a\, dn_a = -2\pi \sin\theta\ \frac{1}{2}\, tg\frac{\theta}{2}\ \Big|_{\theta\to\pi}$$

$$= -\pi\ 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\cdot \sin\frac{\theta}{2}\Big/\cos\frac{\theta}{2} = -2\pi$$

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

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 discribe 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

$$\langle \psi_L^{(2)} \,|\, \frac{d}{dt} \,|\, \psi_L^{(2)} \rangle = \frac{1}{2(1-n_3)} \left[(n_1 + i n_2)(\dot{n}_1 - i\dot{n}_2) + (1-n_3)(-)\dot{n}_3 \right]$$

$$+ \frac{1}{4(1-n_3)^2} \left[(n_1^2 + n_2^2)\,\dot{n}_3 + (1-n_3)^2\,\dot{n}_3 \right]$$

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

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

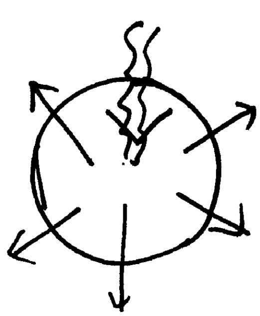
$$\tilde{A}_1 = \frac{n_2}{2(1-n_3)} = \frac{\sin\theta \sin\varphi}{2(1-\cos\theta)} = \frac{\sin\varphi}{2} \operatorname{ctg}\frac{\theta}{2}$$

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

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

the singular point is at the north pole.

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



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

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

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_α is well-defined in northern hemisphere $\Big\}$ ⇐ locally

$\tilde{A}$ is well-defined in the south hemisphere $\Big\}$ but not globally

They overlap at the equator, in which

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

At equation $|\psi_L^{(1)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ n_1 + i n_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\varphi} \end{pmatrix} = e^{-i\varphi}|\psi_u^{(1)}\rangle$

$$|\psi_L^{(2)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} n_1 - i n_2 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\varphi} \\ 1 \end{pmatrix}$$

ω is also the group space of $U(1)$

This map 's the equator $S^1 \longrightarrow U(1)$ group space.

We can define the winding number C_1

$$2\pi C_1 = i \oint_{S_1} \omega^{-1}\partial_\alpha \omega \, dn_\alpha$$

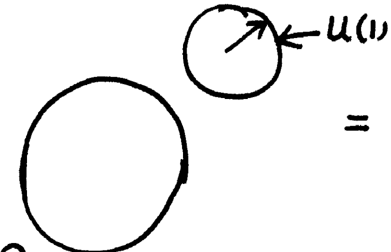
$$2\pi C_1 = \oint_{S_1} A^a dn_a - \oint_{S_1} \tilde{A}^a dn_a$$

$$= \underset{\text{north}}{\iint} d\vec{S} \cdot \vec{B} + \underset{\text{south}}{\iint} d\vec{S} \cdot \vec{B} = \oiint d\vec{S} \cdot \vec{B}$$

Winding number

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

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



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

S_1 equation

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

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

angle is multiple valued.

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

$\boxed{\text{the first Chern number!}}$

For the Low energy level $C_1 = 1$.

Similary, 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.

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

§ Sum-rule of Berry curvature

$$F^n_{\mu\nu}(\vec{R}) = \frac{\partial}{\partial R_\mu} A^n_\nu(R) - \frac{\partial}{\partial R_\nu} A^n_\mu(R) = i\{\langle \frac{\partial}{\partial R_\mu}\psi^n | \frac{\partial}{\partial R_\nu}\psi^n\rangle - \langle \frac{\partial}{\partial R_\nu}\psi^n | \frac{\partial}{\partial R_\mu}\psi^n\rangle\}$$

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

$$\boxed{\sum_n F^n_{\mu\nu}(\vec{R}) = 0}$$

Proof: Let us denote the basis $\psi_n(\vec{R})$ $n=1,2,\cdots$ 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

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

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

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

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

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

$\Rightarrow$ sum to zero.