# ② Parallel transport in quantum mechanics

## 2.1 Berry phase

$\mathcal{H}(\vec{R})$ , where

$$\vec{R} = (R_1, R_2, \dots, R_N)$$

$$\mathcal{H}(\vec{R}) \, |n, \vec{R}\rangle = E_n(\vec{R}) \, |n, \vec{R}\rangle$$

$\{ |n, \vec{R}\rangle \}$ : smooth basis

Vary $\vec{R}$ adiabatically in time :

$t : 0 \to T$

Path $C$.

Note: $C$ can be an open or a closed path.

Initial state:

$$|\psi(0)\rangle = |n, \vec{R}(0)\rangle$$

$$|\psi(T)\rangle = e^{i(\delta_n + \gamma_n)} |\psi(0)\rangle$$

$\delta_n$ = dynamical phase

$\gamma_n$ = Berry phase

$$= i \int_0^T dt \langle n, \vec{R}(t)| \frac{d}{dt} |n, \vec{R}(t)\rangle$$

$$\boxed{= i \int_C \langle n, \vec{R}| \frac{d}{d\vec{R}} |n, \vec{R}\rangle \cdot d\vec{R}}$$

$\gamma_n \in \mathbb{R}$

Proof:

$$n, \vec{R} \Rightarrow x$$

$$\left\langle x \,\middle|\, \frac{dx}{dt} \right\rangle^* =$$

$$= \left\langle \frac{dx}{dt} \,\middle|\, x \right\rangle$$

$$= \frac{d}{dt}\Big( \underbrace{\langle x | x \rangle}_{1 \text{ for all } t} \Big)$$

$$- \left\langle x \,\middle|\, \frac{dx}{dt} \right\rangle$$

$$= - \left\langle x \,\middle|\, \frac{dx}{dt} \right\rangle$$

$\Rightarrow \left\langle x \,\middle|\, \frac{dx}{dt} \right\rangle$ is purely imaginary $\Rightarrow \gamma_n \in \mathbb{R}$

## 2.2 Berry connection

$$\boxed{\vec{A}_n(\vec{R}) \equiv i \langle n, \vec{R} | \frac{d}{d\vec{R}} | n, \vec{R} \rangle}$$

If $\vec{R} = (R_1, R_2, \cdots, R_N)$,

then $\vec{A}_n$ is a $N$-component

vector.

Then,

$$\boxed{\gamma_n = \int_C \vec{A}_n(\vec{R}) \cdot d\vec{R}}$$

$$e^{i\gamma_n} = e^{i\int_C \vec{A}_n \cdot d\vec{R}}$$

Analogy w/ electromagnetism :

charged particle moving in the presence of a vector potential along a path C, its wavefunction acquires a phase

$$e^{\frac{iq}{\hbar}\int_C \underbrace{\vec{A}}_{\text{EM vector potential}} \cdot\, d\underbrace{\vec{r}}_{\text{real space}}}$$

$$e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} = e^{\frac{i}{\hbar}\int_0^{\vec{r}} \vec{p}\cdot d\vec{r}\,'}$$

$$\vec{p} \to \vec{p} + q\vec{A}$$

Extra phase $\quad e^{\frac{i}{\hbar} q \int_0^{\vec{r}} \vec{A}(\vec{r}\,') \cdot d\vec{r}\,'}$

Analogy:

$$\begin{cases} \vec{A}_n(\vec{R}) \longleftrightarrow \vec{A}(\vec{r}) \\ \vec{R} \longleftrightarrow \vec{r} \end{cases}$$

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Consider a "gauge transformation":

$$\boxed{\widetilde{|n, \vec{R}\rangle} = e^{i \varphi_n(\vec{R})} |n, \vec{R}\rangle}$$

$$\tilde{\vec{A}}_n = i\, \widetilde{\langle n, \vec{R}|} \frac{d}{d\vec{R}} \widetilde{|n, \vec{R}\rangle}$$

$$= \boxed{\vec{A}_n + \frac{d}{d\vec{R}} \varphi_n(\vec{R})}$$

Same transformation as vector potential in EM.

Consider

$$i\hbar \frac{\partial \psi}{\partial t} = \left[ \frac{1}{2m} (\vec{p} - q\vec{A})^2 + V(\vec{r}) \right] \psi$$

Define $\tilde{\psi} \equiv \psi e^{i\varphi}$.

It follows that

$$i\hbar \frac{\partial \tilde{\psi}}{\partial t} = \left[ \frac{1}{2m} (\vec{p} - q\vec{\tilde{A}})^2 + V(\vec{r}) \right] \tilde{\psi}$$

with

$$\vec{\tilde{A}} = \vec{A} + \frac{d\varphi}{d\vec{r}}$$

Change of the Berry phase under a gauge transformation:

$$\Delta \gamma_n \equiv \int_C \vec{\tilde{A}}_n(\vec{R}) \cdot d\vec{R}$$

$$- \int_C \vec{A}_n(\vec{R}) \cdot d\vec{R}$$

$$= \int_C \frac{d\varphi_n(\vec{R})}{d\vec{R}} \cdot d\vec{R}$$

$$\vec{\tilde{A}} = \vec{A} + \frac{d\varphi}{d\vec{R}}$$

$$= \varphi_n(\vec{R}(T)) - \varphi_n(\vec{R}(0))$$

For open paths $[\ \vec{R}(T) \neq \vec{R}(0)]$

$$\varphi_n(\vec{R}(T)) - \varphi_n(\vec{R}(0))$$

can be anything.

$\Rightarrow \gamma_n$ is not gauge-invariant for open paths $\Rightarrow$ not physically observable.

For closed paths $[\ \vec{R}(T) = \vec{R}(0)]$,

$$\varphi_n(\vec{R}(T)) = \varphi_n(\vec{R}(0)) \mod 2\pi$$

$$e^{i 2\pi} = 1$$

N.B: we require that

$\{ \widetilde{|n, \vec{R}\rangle} \}$ be single-valued.

Then $e^{i \Delta \gamma_n} = e^{i 2\pi n}$

$n \in \mathbb{Z}$

$= 1$

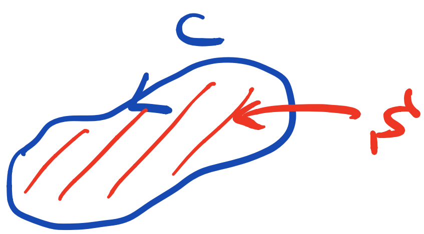
$\Rightarrow e^{i \gamma_n}$ is gauge-invariant for closed loops $\Rightarrow$ potentially observable.

Analogy in EM:

$\int_C \vec{A} \cdot \vec{dr}$ gauge-invariant if C is a closed loop.

Indeed,

$$\oint_C \vec{A}\cdot d\vec{r} \overset{\text{Stokes thm}}{=} \int_S \underbrace{\left(\vec{\nabla}\times\vec{A}\right)}_{\substack{\text{magnetic}\\ \text{field } \vec{B}}}\cdot d\vec{s}$$




$\vec{B}$ is gauge-invariant

because
$$\vec{\nabla}\times\vec{A} = \vec{\nabla}\times\left(\vec{A}+\frac{d\varphi}{d\vec{r}}\right)$$

There's an analogue of magnetic field for the Berry phase.

## 2.3 Berry curvature

$\vec{R} = (R_1, R_2, \dots, R_N)$

$N$ - dimensional parameter space.

Consider a 2D surface $S$, which is bound by the path $C$.

Parametrise the surface with 2 coordinates $(X_i, X_j)$.

ex: if $S$ is a region of the surface of a sphere,

$$(X_i, X_j) = (\theta, \phi)$$

Then, Stokes' thm gives

$$\gamma_n(C) = \oint_C \vec{A}_n(\vec{R}) \cdot d\vec{R}$$

$$= \int_S B_{ij,n}(\underbrace{\vec{X}}_{(X_i,\, X_j)})\, dX_i\, dX_j$$

if the surface has no holes.

where

$$\boxed{B_{ij,n}(\vec{X}) \equiv \left( \frac{\partial A_{j,n}}{\partial X_i} - \frac{\partial A_{i,n}}{\partial X_j} \right)}$$

"Berry curvature" tensor

$\Bigg\{$ real
anti-symmetric under $i \leftrightarrow j$

$B_{ij}$ is gauge-invariant.

$$\tilde{B}_{ij} = B_{ij}$$

Question: we showed that

$$\left.\begin{aligned} \tilde{\gamma}_n &= \gamma_n + 2\pi n_{\in \mathbb{Z}} \\ \tilde{B}_{ij} &= B_{ij} \end{aligned}\right\} \text{ how}$$

to reconcile this?

Another (popular) way of writing $B_{ij,n}$:

$$\boxed{\begin{aligned} & B_{ij,n}(\vec{X}) = \\ & = \underset{\text{complex \#}}{i} \left[ \frac{\partial \langle n, \vec{X}|}{\partial X_i} \frac{\partial |n, \vec{X}\rangle}{\partial X_j} - (i \leftrightarrow j) \right] \end{aligned}}$$

This allows to prove that

$$\boxed{\sum_n B_{n,ij} = 0}$$

$$\Rightarrow \boxed{\sum_n \gamma_n = 0 \mod 2\pi}$$

$\Rightarrow$ need at least 2
-dimensional Hilbert
space in order to have
a nonzero Berry phase.

Proof of $\sum_n B_{n,ij} = 0$ :

$$B_{n,ij} = i \sum_m \Bigg[ \frac{\partial \langle n, \vec{x}|}{\partial x_i} \underbrace{|m, \vec{x}\rangle \langle m, \vec{x}|}_{} \frac{\partial}{\partial x_j} |n, \vec{x}\rangle - (i \leftrightarrow j) \Bigg]$$

$$\sum_m |m, \vec{x}\rangle\langle m, \vec{x}| = 1$$

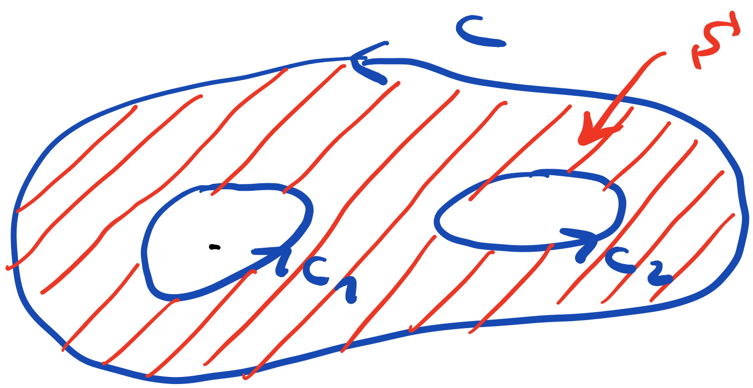
$$= i \sum_m \Bigg[ - \langle n, \vec{x}| \frac{\partial}{\partial x_i} |m, \vec{x}\rangle \langle m, \vec{x}| \frac{\partial}{\partial x_j} |n, \vec{x}\rangle$$

$$+ \langle n, \vec{x}| \frac{\partial}{\partial x_j} |m, \vec{x}\rangle \langle m, \vec{x}| \frac{\partial}{\partial x_i} |n, \vec{x}\rangle \Bigg]$$

Now it's clear that

$$\sum_m B_{ij,m} = 0 .$$

What if the surface $S$ has holes in it?




In this case,

$$\boxed{\gamma_m(C) = \int_S B_{ij,m}(\vec{X})\, dX_1\, dX_2 + \sum_{K} N_K(C)\, \gamma_m(C_K)}$$

hole index

where

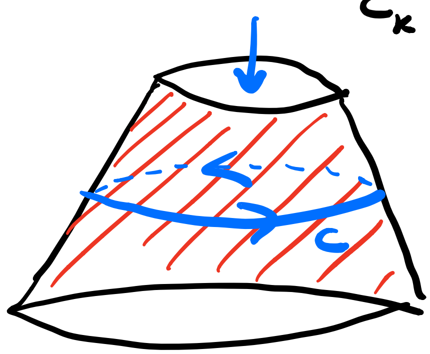
$N_k(c)$ = winding # of $c$ around hole $k$

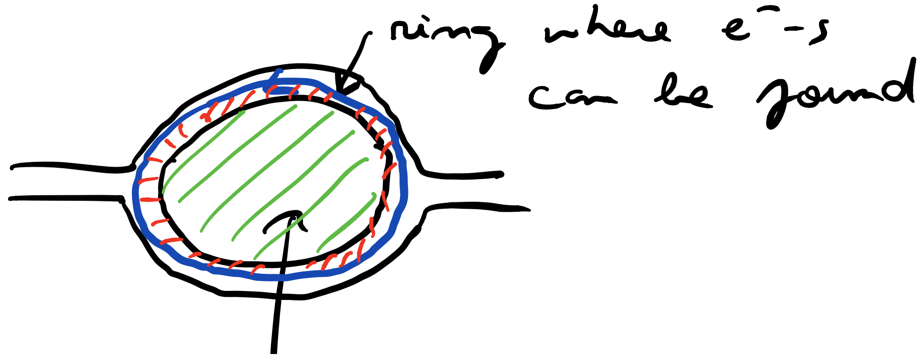
= # of $\circlearrowleft$ turns

− # of $\circlearrowright$ turns

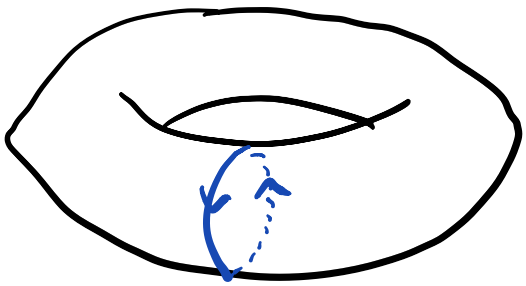
that $c$ makes around hole $k$.

$$\gamma_n(c_k) \equiv \oint_{c_k} \vec{A}_n \cdot d\vec{R}$$



hole.



The preceding expressions become simpler when $\vec{R} = (R_1, R_2, R_3)$.

Then,

$$\gamma_m(C) = \int_S \underbrace{\vec{B}_m(\vec{X})} \cdot d\vec{S}$$

$$+ \sum_K N_K(C)\, \gamma_m(C_K)$$

where

$$\boxed{\vec{B}_n(\vec{X}) = \frac{\partial}{\partial \vec{X}} \times \vec{A}_n(\vec{X})}$$

Berry curvature vector.

Calculational issue with the Berry phase:

$$\frac{\partial |n, \vec{R}\rangle}{\partial R_1} =$$

$$= \frac{|n, \vec{R} + dR\hat{e}_1\rangle - |n, \vec{R}\rangle}{dR}$$

A computer can give very different phase factors for $|n, \vec{R}\rangle$ and $|n, \vec{R} + dR\,\hat{e}_1\rangle$

and that's bad.

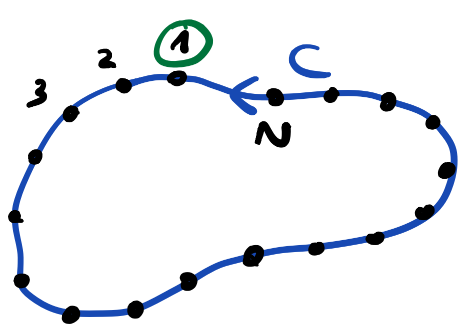
Solutions:

(1) In 3D parameter space:

$$\boxed{\vec{B}_n(\vec{R}) = i \sum_{\substack{m \\ (m \neq n)}} \frac{\langle n, \vec{R} | \frac{\partial \mathcal{H}}{\partial \vec{R}} | m, \vec{R}\rangle \times (n \leftrightarrow m)}{\left[E_n(\vec{R}) - E_m(\vec{R})\right]^2}}$$

vector product

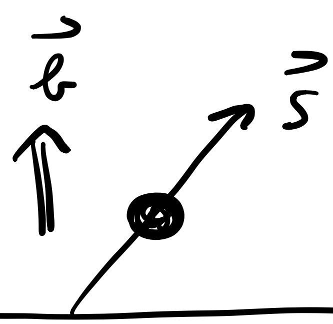
(2) Valid generally



$$\gamma_n = -\,\mathrm{Im}\,\ln\Big[\langle n,\vec{R}_1|\underbrace{n,\vec{R}_2\rangle\langle n,\vec{R}_2}|n,\vec{R}_3\rangle \,\ldots\ldots\, \langle n,\vec{R}_N|n,\vec{R}_1\rangle\Big]$$

## 2.4 Example

Spin $S$ particle in a magnetic field $\vec{B}$.




$$\vec{B} = (B_x, B_y, B_z)$$

$$\boxed{\mathcal{H}(\vec{B}) = -\,\vec{B}\cdot\underbrace{\vec{S}}_{\text{spin operator}}}$$

(absorbed $g\mu_B$ in $\vec{b}$)

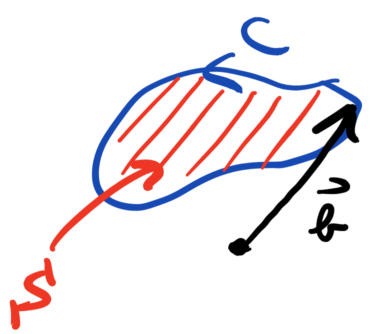
$\vec{b}$ plays the role of $\vec{R}$.

Eigenvalues of $\mathcal{H}$ : $E_n(\vec{b})$

Eigenvectors of $\mathcal{H}$ : $|n, \vec{b}\rangle$

$$n = \underbrace{-S, -S+1, \dots, S-1, S}_{2S+1 \text{ values}}$$

Suppose that $\vec{b}$ is varied slowly along a closed path $C$ :



$$|\psi(0)\rangle = |\underline{\underline{n}}, \vec{R}(0)\rangle$$

$$\underline{\underline{|\psi(T)\rangle}} = e^{i(\delta_n + \gamma_n)} |\underline{\underline{n}}, \vec{R}(T)\rangle$$

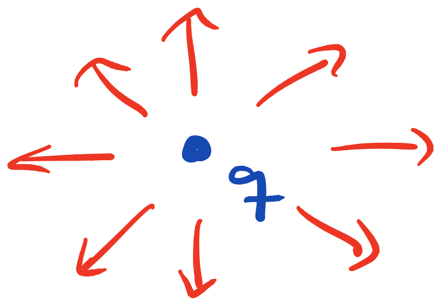
$$\gamma_n = ?$$

$$\gamma_n = \int_{S} \vec{B}_n \cdot d\vec{S}$$

A calculation gives:

$$\boxed{\vec{B}_n = -n \frac{\vec{R}}{R^3}} \Leftarrow$$

Magnetic field created by a magnetic monopole of charge $n$, in parameter space. Monopole is located at $\vec{R} = 0$.




$$\frac{q}{r^2}\hat{r} = \frac{q}{r^3}\vec{r}$$

$\vec{b} = 0$ : degeneracy of $\mathcal{H}$.