I. Review of Berry phase

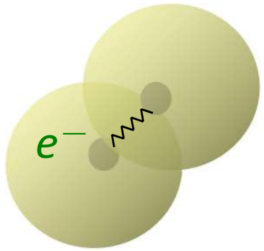
A. Non-degenerate energy level

B. Geometric analogy

C. Degenerate energy levels

System with fast and slow variables

Example: a vibrating H^+_2 molecule,



electron; nuclei

fast ⇕ slow

$$H(\vec{r},\vec{p};\{\vec{R}_i,\vec{P}_i\})$$

Instead of solving the full time-dependent Schroedinger eq., one can use

the Born-Oppenheimer approximation:

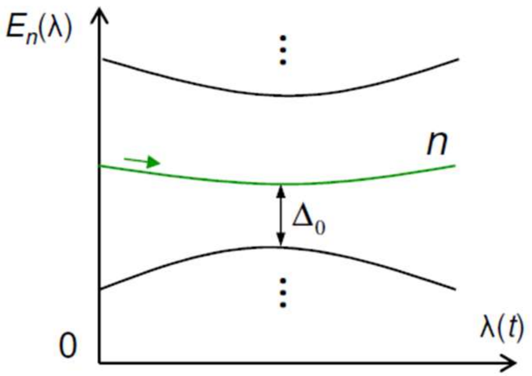
- "Slow variables $\mathbf{R}_i$ are treated as *parameters* $\boldsymbol{\lambda}(t)$
  (the kinetic energies from $\mathbf{P}_i$ are neglected)
- Solve time-independent Schroedinger eq.

$$H(\vec{r},\vec{p};\vec{\lambda})\left|n,\vec{\lambda}\right\rangle = \varepsilon_{n,\vec{\lambda}}\left|n,\vec{\lambda}\right\rangle$$

"snapshot" solution
(single-valued in λ)

Adiabatic evolution of a quantum system

- Energy spectrum



If the characteristic frequency of motion $\Omega_0 \ll \Delta_0/\hbar$, then there is *no* inter-level transition.

(Quantum adiabatic theorem)

$$H_{\boldsymbol{\lambda}}|n, \boldsymbol{\lambda}\rangle = \varepsilon_{n\boldsymbol{\lambda}}|n, \boldsymbol{\lambda}\rangle$$

- After time *t*

$$|\Psi_{n\boldsymbol{\lambda}}(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t dt' \varepsilon_{n\boldsymbol{\lambda}(t')}}|n, \boldsymbol{\lambda}(t)\rangle$$

dynamical phase

- Phases of the snapshot states at different λ's are *independent* and can be assigned arbitrarily

$$\left|n, \vec{\lambda}\right\rangle' = e^{i\gamma_n(\vec{\lambda})}\left|n, \vec{\lambda}\right\rangle$$

Do we need to worry about this phase?

No need!

- Fock, Z. Phys 1928
- Schiff, *Quantum Mechanics* (3rd ed.) p.290

Pf : Consider the *n*-th level,

$$H\left|n,\vec{\lambda}\right\rangle = \varepsilon_{n,\vec{\lambda}}\left|n,\vec{\lambda}\right\rangle$$

snapshot state

$$\left|\Psi_{n\vec{\lambda}}(t)\right\rangle = e^{i\gamma_n(\vec{\lambda})} e^{-i\int_0^t dt'\varepsilon_n(t')}\left|n,\vec{\lambda}\right\rangle$$

$$H\left|\Psi_{n\vec{\lambda}}(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\Psi_{n\vec{\lambda}}(t)\right\rangle$$

$$\Rightarrow \quad \dot{\gamma}_n = i\left\langle n,\vec{\lambda}\right|\frac{\partial}{\partial\vec{\lambda}}\left|n,\vec{\lambda}\right\rangle\cdot\dot{\vec{\lambda}} \neq 0$$

$\equiv$ **$A_n(\lambda)$**

Redefine the phase, $\left|n,\vec{\lambda}\right\rangle' = e^{i\phi_n(\vec{\lambda})}\left|n,\vec{\lambda}\right\rangle$ (ϕ_n is single-valued)

$$\Rightarrow \quad A_n'(\lambda) = A_n(\lambda) - \frac{\partial\phi_n}{\partial\vec{\lambda}}$$

Choose a $\phi(\lambda)$ such that, $A_n'(\lambda)=0$, hence removes this extra phase.

However, there is one problem:

$\nabla_{\vec{\lambda}}\phi = \vec{A}(\vec{\lambda})$ does not always have a (global) well-defined solution!

Two possible cases:

1. $\nabla \times \vec{A} = 0$ everywhere

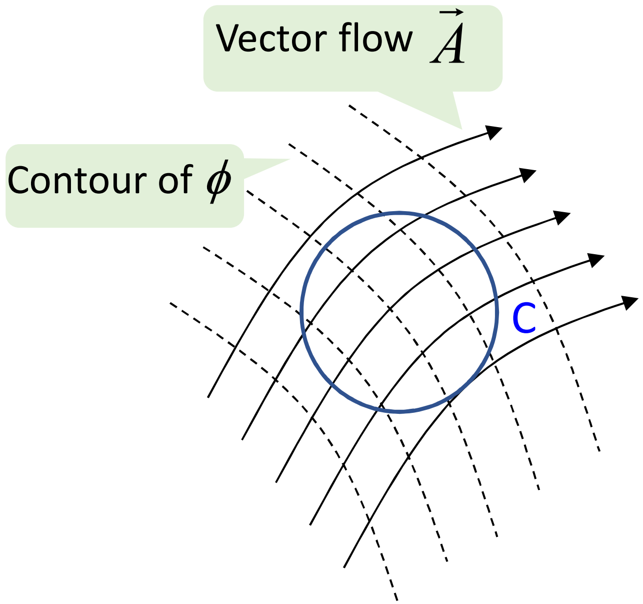
or $\oint_C \vec{A} \cdot d\vec{\lambda} = 0$

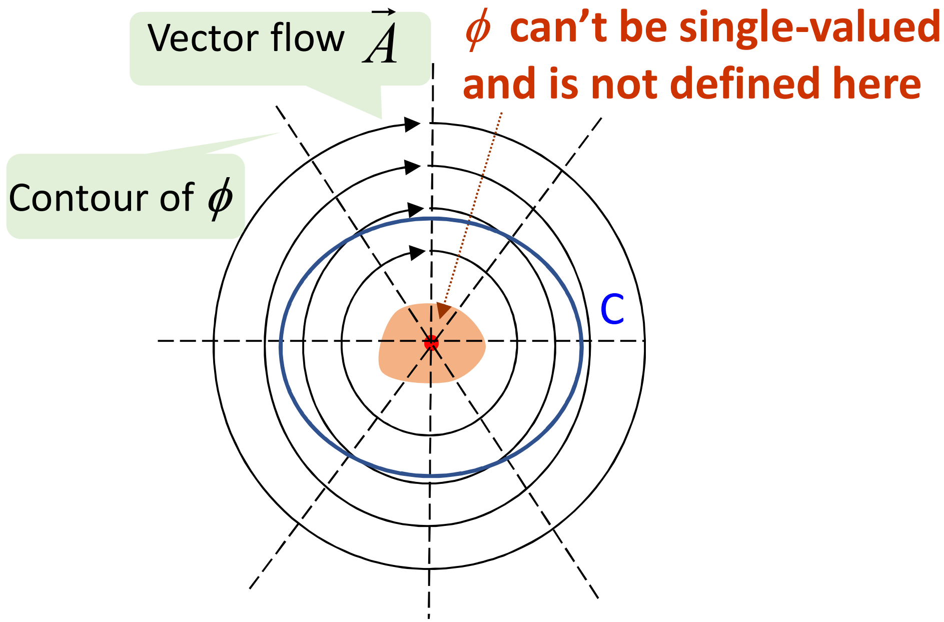
e.g., electrostatic field

2. $\nabla \times \vec{A} \neq 0$ somewhere

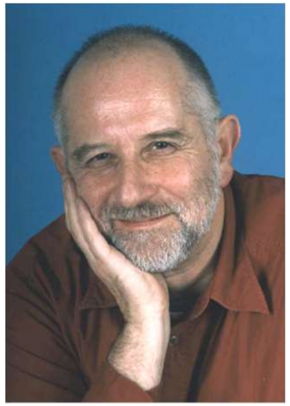
or $\oint_C \vec{A} \cdot d\vec{\lambda} \neq 0$

e.g., vector potential





M. Berry, 1984 :
The parameter-dependent phase is NOT always removable!



For periodic motion with $\lambda(T)=\lambda(0)$, we have, in general

$$\left|\psi_{\vec{\lambda}(T)}\right\rangle = e^{i\gamma_C} e^{-i\int_0^T dt'\varepsilon(t')} \left|\psi_{\vec{\lambda}(0)}\right\rangle$$

Index *n* neglected

- Berry phase (aka geometric phase)

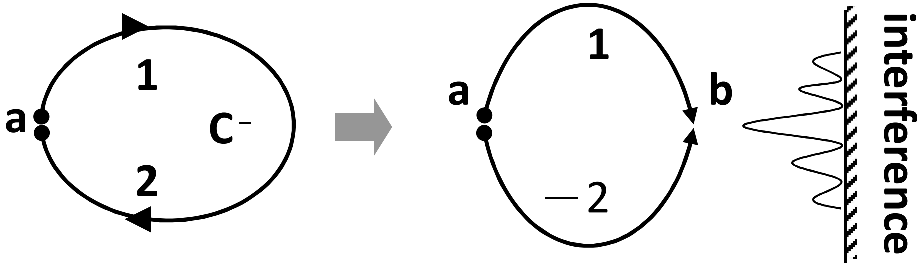
$$\gamma_C = \oint_C \left\langle \vec{\lambda} \right| i \frac{\partial}{\partial \vec{\lambda}} \left| \vec{\lambda} \right\rangle \cdot d\vec{\lambda} \neq 0$$

Depends on the geometry of the path C, independent of the rate $\dot{\gamma}$

- Berry phase is path-dependent

$$\text{if } \oint_C = \int_1 + \int_2 \neq 0, \quad \text{then } \int_1 - \int_{-2} \left(= \int_1 + \int_2 \right) \neq 0$$

Phase difference



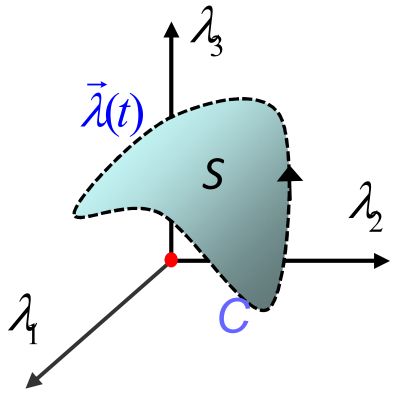
Some terminology

- **Berry connection** (aka Berry potential)

$$\vec{A}(\vec{\lambda}) \equiv i\left\langle \vec{\lambda} \middle| \nabla_\lambda \middle| \vec{\lambda} \right\rangle$$

- **Stokes theorem** (3-dim here, can be higher)

$$\gamma_C = \oint_C \vec{A} \cdot d\vec{\lambda} = \int_S \nabla_{\vec{\lambda}} \times \vec{A} \cdot d\vec{a}$$



- **Berry curvature** (aka Berry field)

$$\vec{F}(\vec{\lambda}) \equiv \nabla_\lambda \times \vec{A}(\vec{\lambda}) = i\left\langle \nabla_\lambda \psi_{\vec{\lambda}} \middle| \times \middle| \nabla_\lambda \psi_{\vec{\lambda}} \right\rangle$$

For a small loop,

$$\gamma_C = \int_S \vec{F} \cdot d\vec{a} \simeq \vec{F} \cdot d\vec{a}$$

- **Gauge transformation**

  - $\left|\psi_{\vec{\lambda}}\right\rangle \rightarrow e^{i\chi(\vec{\lambda})}\left|\psi_{\vec{\lambda}}\right\rangle$
  - $\vec{A}(\vec{\lambda}) \rightarrow \vec{A}(\vec{\lambda}) - \nabla_\lambda \chi$
  - $\vec{F}(\vec{\lambda}) \rightarrow \vec{F}(\vec{\lambda})$
  - $\gamma_C \rightarrow \gamma_C$

Redefine the phases of the snapshot states (χ is single-valued)

Berry curvature and Berry phase are not changed under the G.T.

Analogy with electromagnetism

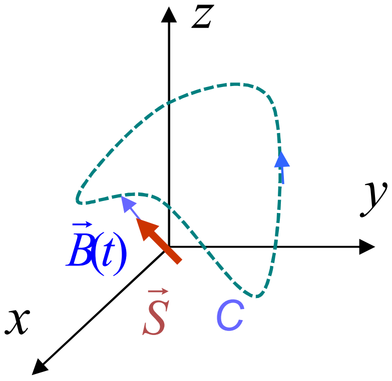
Electromagnetism	Quantum anholonomy
vector potential $\mathbf{A}(\mathbf{r})$	Berry connection $\mathbf{A}(\boldsymbol{\lambda})$
magnetic field $\mathbf{B}(\mathbf{r})$	Berry curvature $\mathbf{F}(\boldsymbol{\lambda})$
magnetic monopole	degenerate point
magnetic charge	Berry index
magnetic flux $\Phi(C)$	Berry phase $\gamma(C)$

(aka monopole charge, topological charge, etc)

A canonical example (we'll cite this result several times later)

A spin-1/2 particle in a *slowly changing B* field

- **Real space**



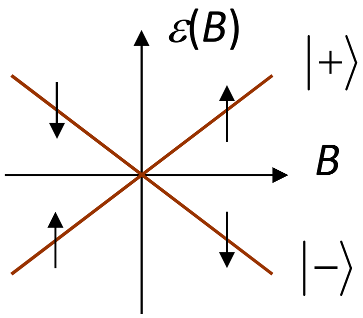
$$H_{\vec{\lambda}=\vec{B}} = \mu_B \vec{B}\cdot\vec{\sigma}$$

- Eingenvalues and eigenstates

$$\varepsilon_\pm = \pm\mu_B B$$

$$|\hat{n},+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix},\ |\hat{n},-\rangle = \begin{pmatrix} -e^{-i\phi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}.$$

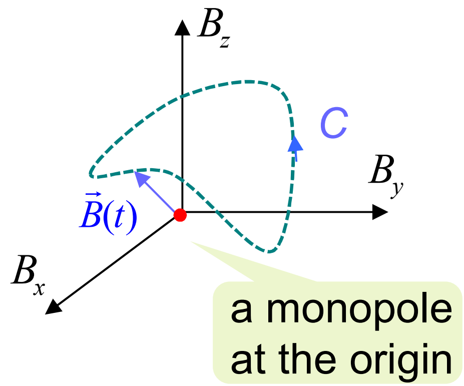
Level crossing at B=0

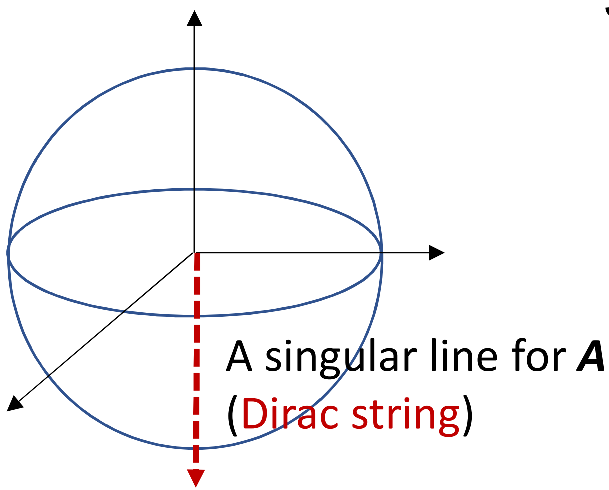


- Different choices of phases (gauge choices)

$|\hat{n},\pm\rangle' = e^{\mp i\phi}|\hat{n},\pm\rangle$ are also single-valued. You can check that $|\hat{n},\pm\rangle$ have ϕ-ambiguity at $\theta=\pi$ (but not at $\theta=0$), while $|\hat{n},\pm\rangle'$ have ϕ-ambiguity at $\theta=0$ (but not at $\theta=\pi$).

- **Parameter space**





- Berry connection

$$\frac{\partial}{\partial \mathbf{B}} = \frac{\partial}{\partial B}\hat{e}_r + \frac{1}{B}\frac{\partial}{\partial\theta}\hat{e}_\theta + \frac{1}{B\sin\theta}\frac{\partial}{\partial\phi}\hat{e}_\phi$$

$$\begin{aligned}\mathbf{A}_+(\mathbf{B}) &= i\langle\mathbf{B},+|\frac{\partial}{\partial\mathbf{B}}|\mathbf{B},+\rangle \\ &= -\frac{1}{2B}\frac{1-\cos\theta}{\sin\theta}\hat{e}_\phi.\end{aligned}$$

~ vector potential of a monopole

Similarly, $\mathbf{A}_-(\mathbf{B}) = \frac{1}{2B}\frac{1-\cos\theta}{\sin\theta}\hat{e}_\phi$

Both $\mathbf{A}_\pm(\mathbf{B})$ are singular along $\theta=\pi$.

(relates to the ϕ-ambiguity)

- Berry curvature

$$\Rightarrow \mathbf{F}_\pm(\mathbf{B}) = \nabla_{\mathbf{B}}\times\mathbf{A}_\pm(\mathbf{B}) = \mp\frac{1}{2}\frac{\hat{B}}{B^2}$$

~ magnetic field of a monopole

Point of level crossing is the source of Berry curvature

- Berry phase

$$\gamma_\pm(C) = \mp\frac{1}{2}\Omega(C)$$

spin × solid angle

- Berry index
  (topological charge)

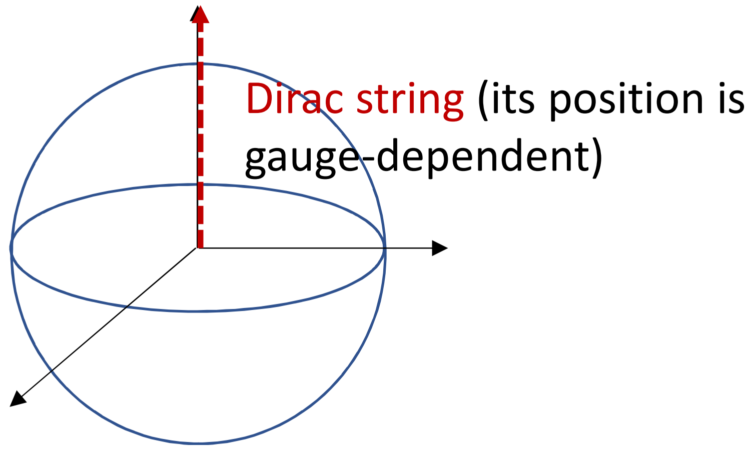
$$\frac{1}{2\pi}\int_{S_B^2} d^2\mathbf{a}\cdot\mathbf{F}_\pm(\mathbf{B}) = \mp 1$$

- Gauge transformation

$$|\hat{n},\pm\rangle' = e^{\mp i\phi}|\hat{n},\pm\rangle$$

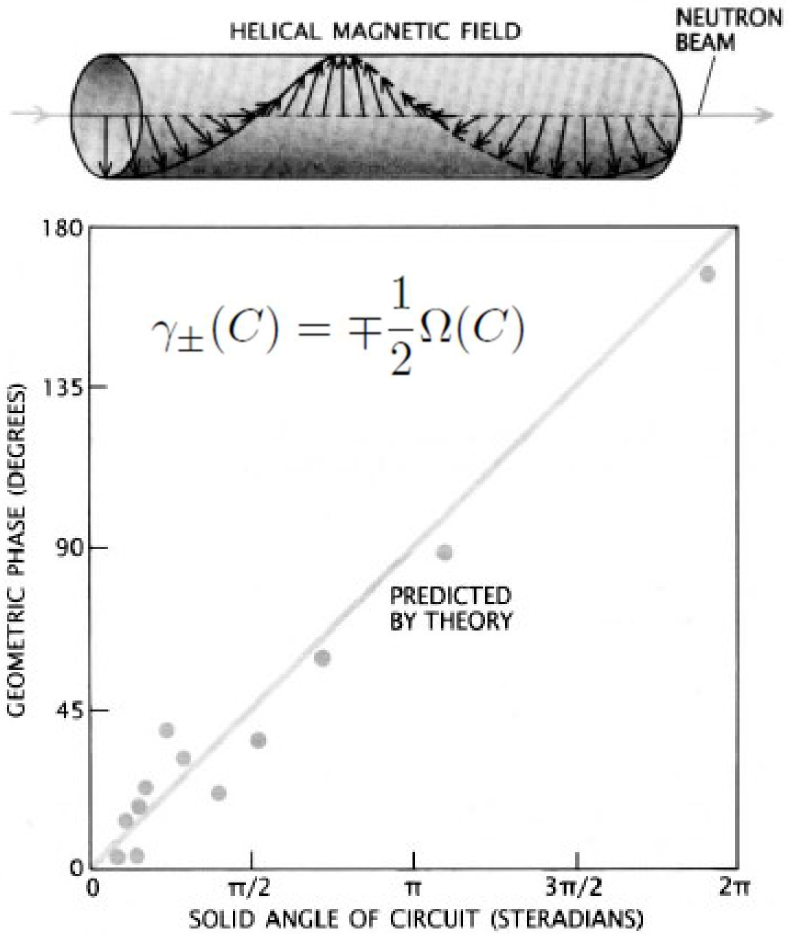
$$\begin{aligned}\mathbf{A}'_\pm(\mathbf{B}) &= \mathbf{A}_\pm(\mathbf{B}) \pm \frac{\partial\phi}{\partial\mathbf{B}} \\ &= \mathbf{A}_\pm(\mathbf{B}) \pm \frac{1}{B\sin\theta}\hat{e}_\phi \\ &= \pm\frac{1}{2B}\frac{1+\cos\theta}{\sin\theta}\hat{e}_\phi\end{aligned}$$

Both $\mathbf{A}'_\pm(\mathbf{B})$ are singular along $\theta = 0$.



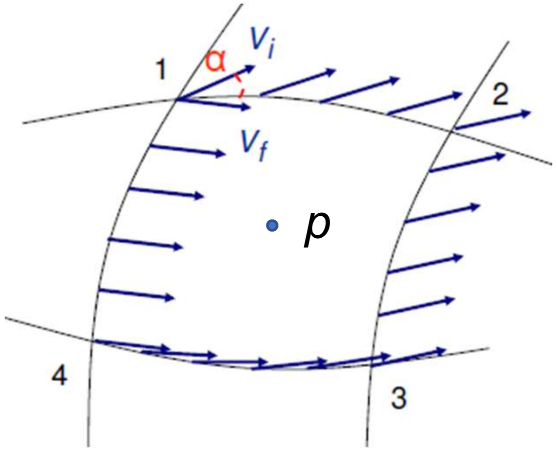
Experiments : Bitter and Dubbers , PRL 1987

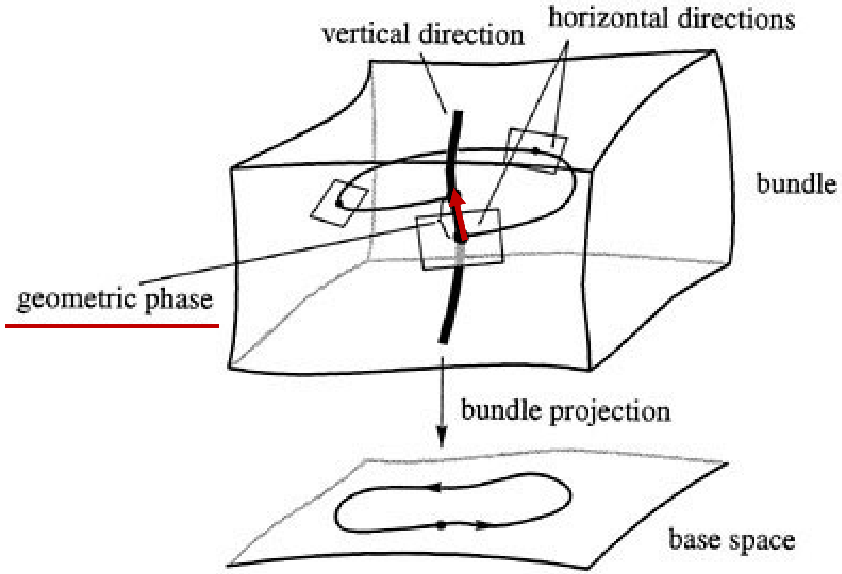
Neutrons fly through a helical magnetic field



Berry phase ~ Anholonomy angle

Fiber bundle = U(1) phase x λ-space





For a small s, $\gamma_C = \int_S \vec{F} \cdot d\vec{a} \simeq \vec{F} \cdot d\vec{a}$

$G \equiv \lim_{A \to 0} \frac{\alpha_A}{A}$ Gaussian curvature

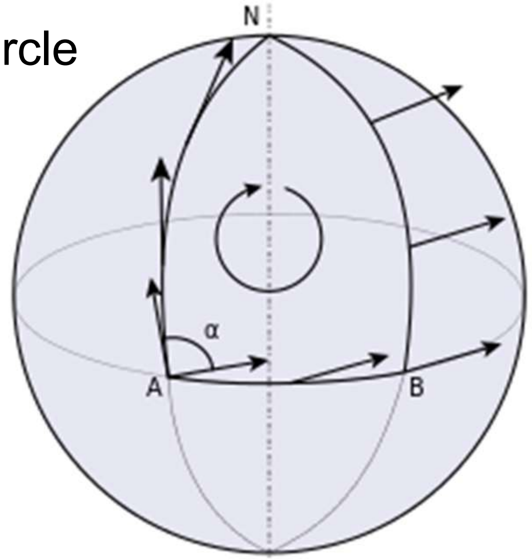
$\vec{\mathrm{F}} \cdot \hat{n} \equiv \lim_{A \to 0} \frac{\gamma_C}{A}$ Berry curvature

Fig. from *Fiber bundles and quantum theory*, by Bernstein and Phillips, Sci. Am. 1981

Revisiting parallel transport (PT)

- PT along a geodesic curve

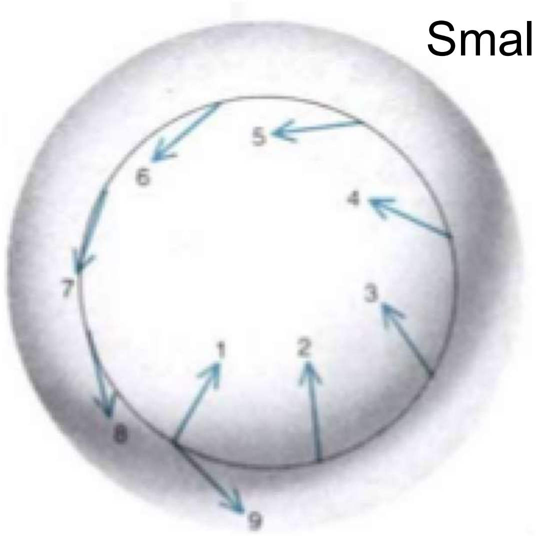
Great circle



$$\alpha_A = \frac{A}{r^2}$$

- PT along a general curve

Small circle



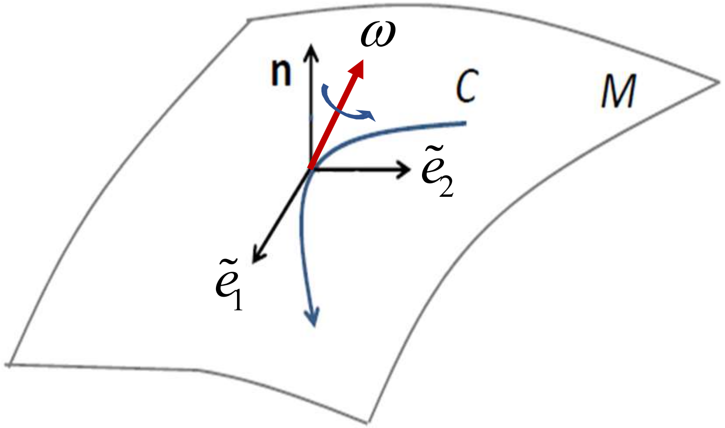
α_A = ?

The earlier definition of PT cannot be right (e.g., transporting a vector along a general curve on a flat surface).

New definition of PT:

v does not twist around the local vertical axis (normal vector **n**) as we move along a curve C.

A moving frame on a curved surface



$$\dot{\tilde{\mathbf{e}}}_1 = \boldsymbol{\omega} \times \tilde{\mathbf{e}}_1$$

$$\begin{aligned} \boldsymbol{\omega} \cdot \mathbf{n} &= \boldsymbol{\omega} \cdot \tilde{\mathbf{e}}_1 \times \tilde{\mathbf{e}}_2 \\ &= \boldsymbol{\omega} \times \tilde{\mathbf{e}}_1 \cdot \tilde{\mathbf{e}}_2 = \dot{\tilde{\mathbf{e}}}_1 \cdot \tilde{\mathbf{e}}_2 = 0 \end{aligned}$$

PT condition

Parallel transport condition of a moving triad $(\boldsymbol{n}, \tilde{e}_1, \tilde{e}_2)$:

No rotation around ***n***,

$$\boldsymbol{\omega} \cdot \mathbf{n} = 0$$

Angular velocity

Define complex vector

$$\psi = \frac{1}{\sqrt{2}} (\tilde{\mathbf{e}}_1 + i\tilde{\mathbf{e}}_2)$$

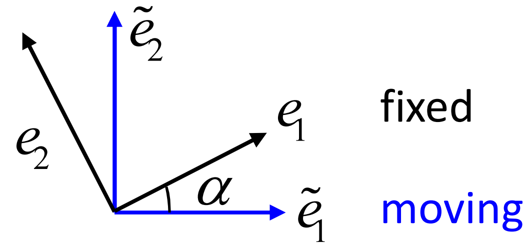
$$\mathrm{Im}\left(\psi^* \cdot \dot{\psi}\right) = 0, \ \text{or} \ \boxed{i\psi^* \cdot \dot{\psi} = 0.}$$

Alternative form of the PT condition

PT frame *vs* fixed frame:

fixed triad $(\boldsymbol{n}, e_1, e_2)$

moving triad $(\boldsymbol{n}, \tilde{e}_1, \tilde{e}_2)$



define $\phi = \frac{1}{\sqrt{2}}(\mathbf{e}_1 + i\mathbf{e}_2)$

$$\psi = \frac{1}{\sqrt{2}}(\tilde{\mathbf{e}}_1 + i\tilde{\mathbf{e}}_2)$$

then $\psi(\mathbf{r}) = \phi(\mathbf{r})e^{i\alpha(\mathbf{r})}$

➡ $\psi^* \cdot d\psi = \phi^* \cdot d\phi + id\alpha$

➡ $\alpha(C) = i\oint_C \phi^* \cdot \frac{d\phi}{d\mathbf{r}} \cdot d\mathbf{r}$ versus $i\psi^* \cdot \dot{\psi} = 0$

PT condition

Fixed states, single-valued

PT states, not single-valued

Analogy: $\gamma(C) = i\oint_C \langle \phi_{\vec{\lambda}} | \nabla_\lambda \phi_{\vec{\lambda}} \rangle \cdot d\vec{\lambda}$ ⬌ $i\langle \psi_{\vec{\lambda}} | \nabla_\lambda \psi_{\vec{\lambda}} \rangle = 0$

Snapshot states

PT states

Analogy

	geometry	quantum state
fixed basis	$\phi(x)$	$\lvert\phi;\boldsymbol{\lambda}\rangle$
PT basis	$\psi(x)$	$\lvert\psi;\boldsymbol{\lambda}\rangle$
PT condition	$i\psi^* \cdot \dot{\psi} = 0$	$i\langle\psi\lvert\dot{\psi}\rangle = 0$
holonomy	anholonomy angle	Berry phase
curvature	Gaussian curvature	Berry curvature
topological number	Euler characteristic	Chern number

$$\chi = \frac{1}{2\pi}\int_S da\, G \qquad C = \frac{1}{2\pi}\int_M d\vec{a}\cdot\vec{F}$$

陳省身
(1911-2004)

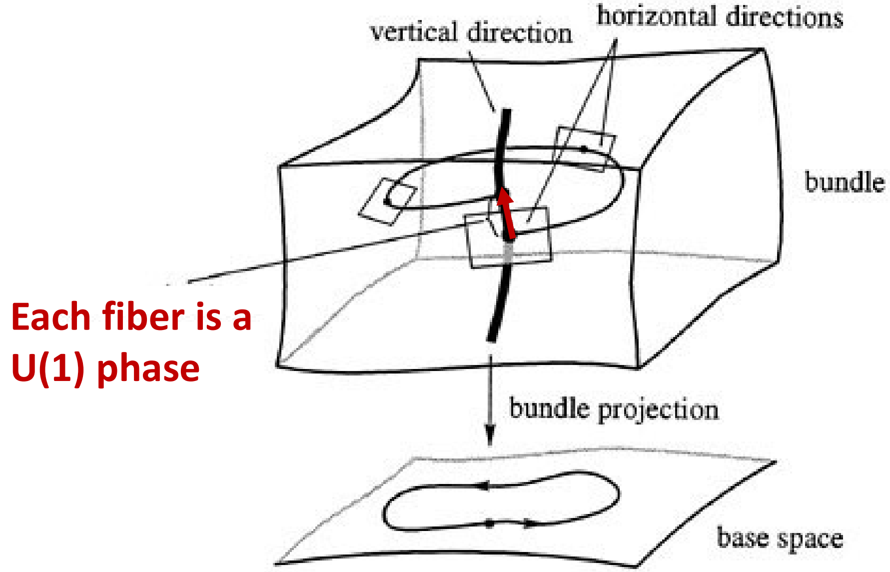
C. Degenerate energy levels

- Non-degenerate level

Wave function is a scalar

$$\left|\psi_{\vec{\lambda}(T)}\right\rangle = e^{i\gamma_C} e^{-i\int_0^T dt'\varepsilon(t')} \left|\psi_{\vec{\lambda}(0)}\right\rangle$$

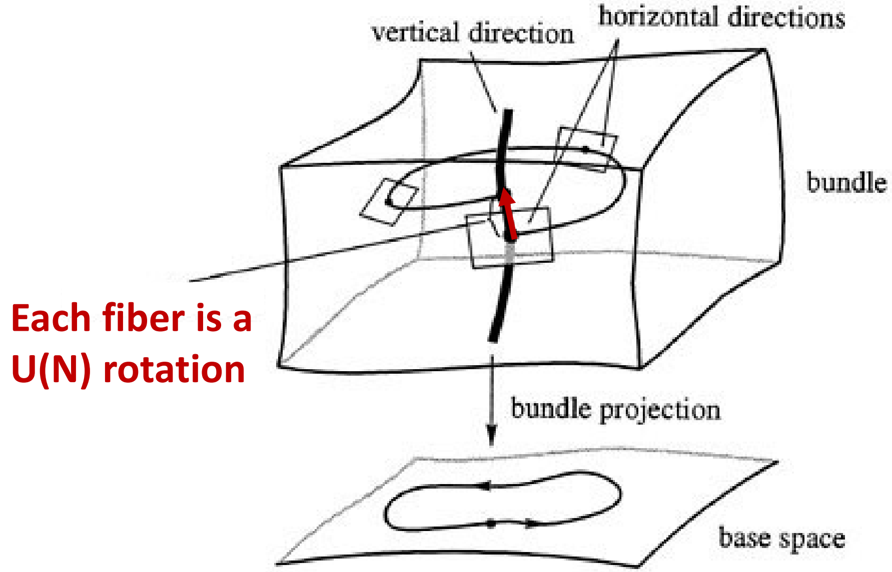
Initial state and final state differ by a U(1) phase



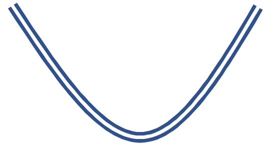
- Degenerate levels (N-fold degeneracy)

Wave function is a N-component spinor

Initial state and final state differ by a U(N) rotation.
After diagonalization, you get N U(1) phases



For example, 2-fold degeneracy



$$
\left\{
\begin{aligned}
|\Psi_{n,1}(t)\rangle \;&=\; e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}} \\
&\quad \times \left(|n,1,\boldsymbol{\lambda}(t)\rangle\Gamma_{11}(t) + |n,2,\boldsymbol{\lambda}(t)\rangle\Gamma_{21}(t)\right), \\
|\Psi_{n,2}(t)\rangle \;&=\; e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}} \\
&\quad \times \left(|n,1,\boldsymbol{\lambda}(t)\rangle\Gamma_{12}(t) + |n,2,\boldsymbol{\lambda}(t)\rangle\Gamma_{22}(t)\right).
\end{aligned}
\right.
$$

or

$$
|\Psi_{n\beta}(t)\rangle = \underbrace{e^{-\frac{i}{\hbar}\int_0^t dt'\varepsilon_{n\boldsymbol{\lambda}(t')}}}_{\text{Dynamical phase}} \sum_{\alpha} |n\alpha\boldsymbol{\lambda}(t)\rangle \underbrace{\Gamma_{\alpha\beta}}_{\textbf{Berry rotation matrix}}(t).
$$

$$\langle\Psi_{n\alpha}|\Psi_{n\beta}\rangle = \delta_{\alpha\beta}$$

➡ $\Gamma^{\dagger}\Gamma = \Gamma\Gamma^{\dagger} = 1$ Unitary rotation, U(2) matrix

$$H|\Psi_{n\beta}(t)\rangle = i\hbar\frac{\partial}{\partial t}|\Psi_{n\beta}(t)\rangle$$

$$\Rightarrow \quad \frac{d\Gamma_{\alpha\beta}}{dt} = -\sum_{\gamma}\langle n\alpha\boldsymbol{\lambda}|\frac{\partial}{\partial t}|n\gamma\boldsymbol{\lambda}\rangle\Gamma_{\gamma\beta}$$

$$= i\sum_{\gamma}\dot{\boldsymbol{\lambda}}(t)\cdot\mathbf{A}^{(n)}_{\alpha\gamma}(\boldsymbol{\lambda})\Gamma_{\gamma\beta},$$

where $\boxed{\mathbf{A}^{(n)}_{\alpha\beta}(\boldsymbol{\lambda}) \equiv i\langle n\alpha\boldsymbol{\lambda}|\frac{\partial}{\partial\boldsymbol{\lambda}}|n\beta\boldsymbol{\lambda}\rangle}$ **Berry connection** (2x2 matrix)

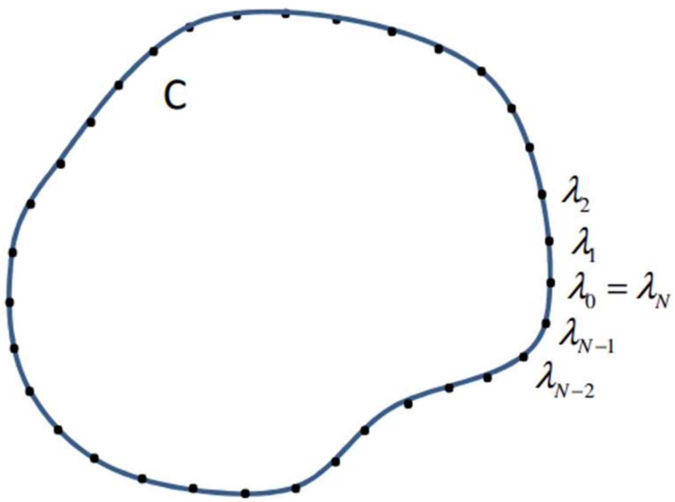
$$\Gamma(t+dt) = \Gamma(t) + idt\dot{\boldsymbol{\lambda}}(t)\cdot\vec{A}(t)\Gamma(t)$$

$$\simeq e^{idt\dot{\boldsymbol{\lambda}}(t)\cdot\vec{A}(t)}\Gamma(t)$$

$$\Rightarrow \quad \Gamma(t) = \cdots e^{id\boldsymbol{\lambda}\cdot\vec{A}(\boldsymbol{\lambda}_1)}e^{id\boldsymbol{\lambda}\cdot\vec{A}(\boldsymbol{\lambda}_0)}\Gamma(0)$$

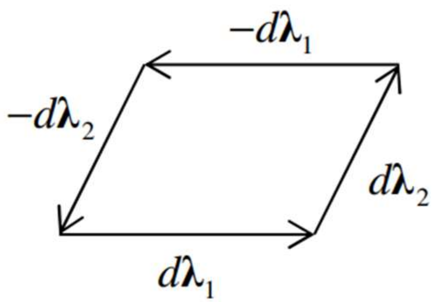
$$\equiv \underline{P}e^{i\int_{\boldsymbol{\lambda}_0}^{\boldsymbol{\lambda}(t)} d\boldsymbol{\lambda}\cdot\vec{A}(\boldsymbol{\lambda})}, \quad \Gamma(0) = 1,$$

path-ordering operator.



Aka Wilson loop

Berry curvature (Berry rotation per unit area)



$$i\vec{\mathsf{F}}_{\Box} \cdot \hat{\mathbf{n}} \equiv \frac{\Gamma_{\Box} - 1}{d^2 a}$$

$$\begin{aligned} &\Gamma_{\Box}(\boldsymbol{\lambda}) \\ = \;& \Gamma(\boldsymbol{\lambda}, \boldsymbol{\lambda} + d\boldsymbol{\lambda}_2)\Gamma(\boldsymbol{\lambda} + d\boldsymbol{\lambda}_2, \boldsymbol{\lambda} + d\boldsymbol{\lambda}_1 + d\boldsymbol{\lambda}_2) \\ \times \;& \Gamma(\boldsymbol{\lambda} + d\boldsymbol{\lambda}_1 + d\boldsymbol{\lambda}_2, \boldsymbol{\lambda} + d\boldsymbol{\lambda}_1)\Gamma(\boldsymbol{\lambda} + d\boldsymbol{\lambda}_1, \boldsymbol{\lambda}) \end{aligned}$$

$$\Rightarrow \quad \mathsf{F}_{k\ell} = \partial_k \mathsf{A}_\ell - \partial_\ell \mathsf{A}_k - i[\mathsf{A}_k, \mathsf{A}_\ell].$$ 2x2 matrix for each *k,l*

non-commutative: Non-Abelian Berry curvature

A 3x3 antisymmetric matrix (with indices k,l) is equivalent to a vector (see latex note for details)

Alternative form: $\mathsf{F}_{k\ell} d\lambda_{1k} d\lambda_{2\ell} = \vec{\mathsf{F}} \cdot d^2\mathbf{a},$

where $$\vec{\mathsf{F}} = \nabla_{\boldsymbol{\lambda}} \times \vec{\mathsf{A}} - i\vec{\mathsf{A}} \times \vec{\mathsf{A}}.$$

2x2 matrix for each vector component