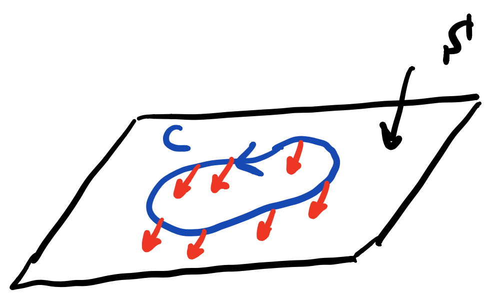
ELEMENTS OF TOPOLOGICAL BAND THEORY

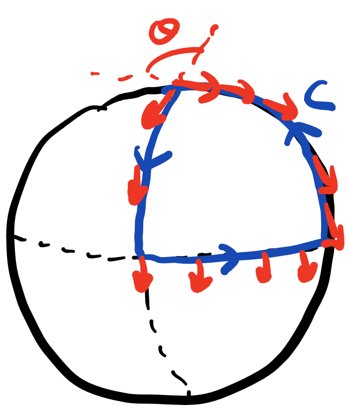
① Parallel transport in geometry

1.1 Holonomy

Parallel transport a vector along a closed loop C on a surface S. The vector rotates by an angle Θ.

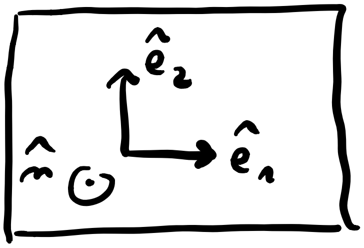


$\Theta = 0$



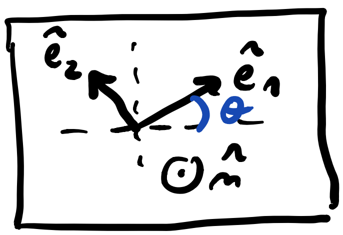
$\Theta = \frac{\pi}{2}$ (for this particular C)

$t = 0$



plane tangent to S

$t = T$



plane tangent to S

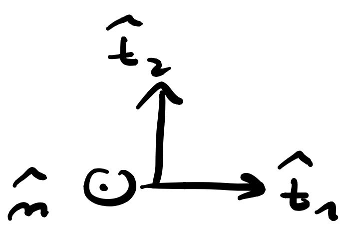
Define $\vec{\phi} \equiv \frac{1}{\sqrt{2}}\left[\hat{e}_1 + i\hat{e}_2\right]$

$$\boxed{\vec{\phi}^* \cdot \dot{\vec{\phi}} = 0} \qquad (1)$$

(law of parallel transport).

Define smooth, single-valued reference system on the surface:

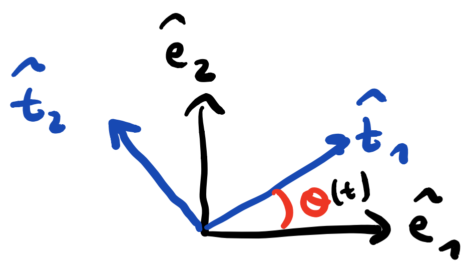
$(\hat{t}_1, \hat{t}_2, \hat{n})$.



e.g. $(\hat{\theta}, \hat{\phi}, \hat{r})$

$$\vec{u} \equiv \frac{1}{\sqrt{2}} \left(\hat{t}_1 + i\,\hat{t}_2 \right)$$

$$\boxed{\vec{\phi} = e^{-i\theta(t)}\,\vec{u}} \qquad (2)$$



$$\dot{\theta} = -i\,\vec{u}^{\,*} \cdot \dot{\vec{u}}$$

$$\boxed{\begin{aligned} \theta &= \mathrm{Im} \int_0^T \vec{u}^{\,*} \cdot \dot{\vec{u}}\,dt \\ &= \mathrm{Im} \oint_c \vec{u}^{\,*} \cdot \underline{d\vec{u}} \end{aligned}} \qquad (3)$$

1.2 Connection and curvature

Choose a coordinate system (X_1, X_2) on S.

Example:

(i) flat surface on the xy plane:

$$(X_1, X_2) = (x, y)$$

(ii) surface of sphere:

$$(X_1, X_2) = (\theta, \phi)$$

Then

$$du_i = \frac{\partial u_i}{\partial \vec{X}} \cdot d\vec{X}$$

where $\vec{X} = (X_1, X_2)$

$$\Rightarrow \theta(c) =$$

$$= \operatorname{Im} \oint_c u_i^*(\vec{x}) \, \frac{\partial u_i(\vec{x})}{\partial \vec{x}} \cdot d\vec{x}$$

(sum over $i = 1, 2, 3$)

Define

$$\boxed{A_i(\vec{x}) \equiv \operatorname{Im}\left[\vec{u}^*(\vec{x}) \cdot \frac{\partial \vec{u}(\vec{x})}{\partial x_i}\right]}$$

i-th component of the "connection"

Then,

$$\boxed{\theta(c) = \oint_c \vec{A}(\vec{x}) \cdot d\vec{x}}$$

The choice of $\hat{t}_1$ is not unique.

$$\underline{\vec{u}'(\vec{x})} = e^{i\alpha(\vec{x})}\,\vec{u}(\vec{x})$$

is an equally valid choice.

" gauge freedom "

$$A_i'(\vec{x}) = A_i(\vec{x}) - \frac{\partial \alpha}{\partial x_i}$$

However,

$$\theta'(c) = \oint_c \vec{A}'(\vec{x}) \cdot d\vec{x}$$

$$= \theta(c) - \oint_c \frac{\partial \alpha}{\partial \vec{x}} \cdot d\vec{x}$$

$$= \theta(c) - \Big[\underbrace{\alpha_{final} - \alpha_{initial}}_{\text{zero for a single-valued ref. system}}\Big]$$

$\Rightarrow \theta(C)$ is "gauge-invariant"

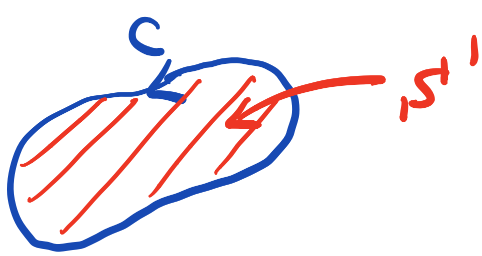
An alternative understanding of $\theta(C)$:

$$\theta(C) = \oint_C \vec{A}(\vec{X}) \cdot d\vec{X}$$

$$= \int_{S'} B(\vec{X})\, dX_1\, dX_2$$

Stokes' thm

simply connected surface (no holes)



where

$$B(\vec{X}) = \left(\frac{\partial A_2}{\partial X_1} - \frac{\partial A_1}{\partial X_2} \right)$$

$\downarrow$

"gauge-invariant"

Geometric meaning of $B(\vec{X})$:

$$B(\vec{X})\, dX_1\, dX_2 \equiv \underbrace{K}\ \underbrace{dS'}$$

Gaussian curvature

(sphere: $\frac{1}{R^2}$)

infinitesimal area element

(sphere: $R^2 \sin\theta\, d\theta\, d\phi$)

For a sphere,

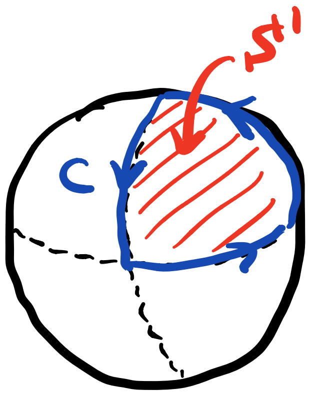
$$\int_{S'} B(\vec{X})\, dX_1\, dX_2 = \Theta(C) =$$

$$= \int_{S'} d\theta \sin\theta\, d\phi$$

$= $ solid angle subtended by C at the center of sphere.

$\equiv \Omega(C)$

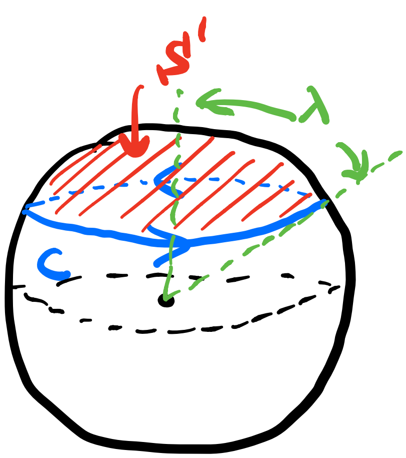
Examples:



$\Omega(C) =$

$$= \int_0^{\pi/2} d\phi \int_0^{\frac{\pi}{2}} d\theta \sin\theta$$

$$= \frac{\pi}{2}$$



$\Theta(C) = \Omega(C)$

$$= \int_0^{2\pi} d\phi \int_0^{\lambda} d\theta \sin\theta$$

$$= 2\pi (1 - \cos\theta)$$

$$\boxed{\Theta(C) = \Omega(C)}$$

holds also for non-spherical surfaces.

Method:

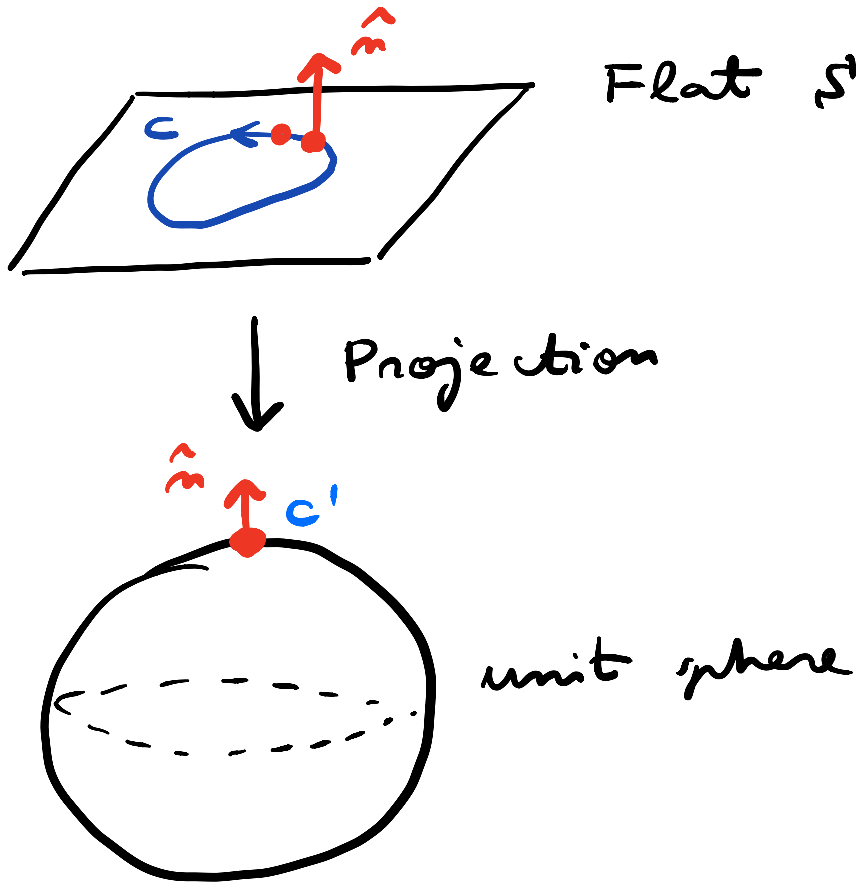
"Project" C defined in S to C' on the surface of a sphere of unit radius.

How?

A point in C with a normal vector $\hat{n}$ is mapped onto a point on the surface of the sphere having the <u>same</u> $\hat{n}$.

Then, $\Theta(c) = \Omega(c')$

Trivial example: (reality check)

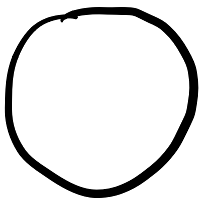


$\Omega(c') = 0 \Rightarrow \Theta(c) = 0$

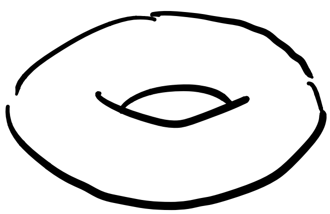
1.3 Gauss-Bonnet theorem

S : closed surface

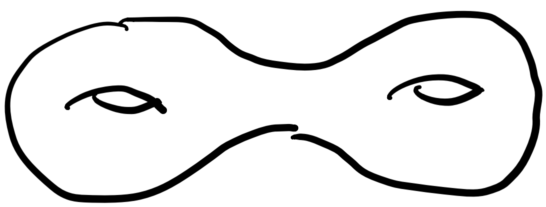
(possibly w/ holes)



$g = 0$



$g = 1$



$g = 2$

$g =$ "genus"

$$\boxed{\oint_{S^1} B(\vec{X})\, dX_1\, dX_2 = 4\pi(1-g)}$$

g = topological invariant.

Analogous invariants arise in quantum physics.

2 Parallel transport in quantum mechanics

2.1 Berry phase

Hamiltonian $\mathcal{H}$ that depends on external parameters

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

electric fields, magnetic fields, positions of nuclei (if we're interested in the electronic Hamiltonian, crystal momentum in a solid)

For each $\vec{R}$,

$$\mathcal{H}(\vec{R}) \underbrace{|n, \vec{R}>}_{\text{eigenvector}} = \underbrace{E_n(\vec{R})}_{\text{eigenvalue}} |n, \vec{R}>$$

n = eigenvalue index.

Suppose that all $E_n(\vec{R})$ are non-degenerate.

Closed loop in parameter space:

$$C \equiv \{ \vec{R}(t) \mid t = 0 \to T \}$$

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

$$E_n(\vec{R}(0)) = E_n(\vec{R}(T))$$

$$|n, \vec{R}(0)\rangle = |n, \vec{R}(T)\rangle \quad]$$

we assume that

$\{ |n, \vec{R}\rangle \}$ is a

singled-valued basis.

$|n, \vec{R}\rangle$ is defined modulo

a phase.

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

is an equally valid eigenstate.

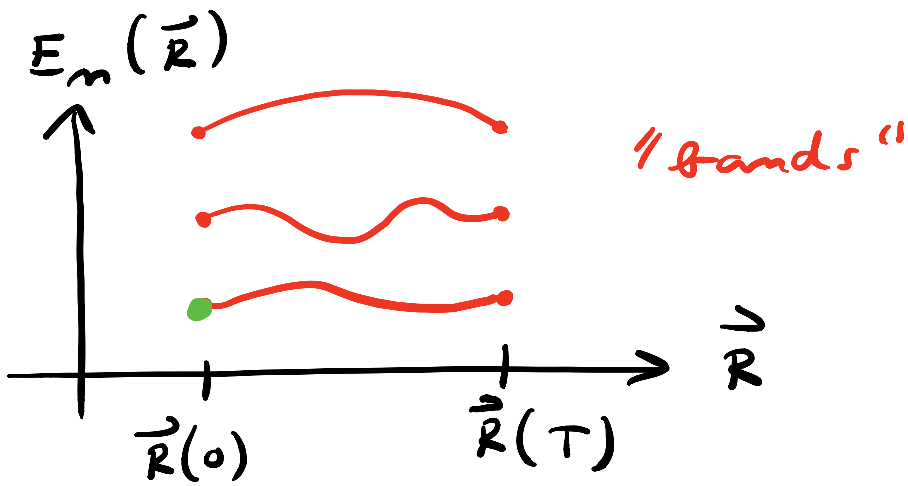
"gauge freedom"

In principle, $\varphi_n(\vec{R})$ can be arbitrary. It can also vary wildly from one $\vec{R}$ to another.

We want $\{|n, \vec{R}\rangle\}$ to be smooth basis + single-valued.

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

If $|n, \underbrace{\vec{R}(0)}\rangle = e^{i\varphi}|n, \underbrace{\vec{R}(T)}\rangle$



$\vec{R}$ is changed "adiabatically" in time.

$\Rightarrow$ "<u>Adiabatic theorem</u>":

Prepare an initial state

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

Then, under time evolution,

$$|\psi(t)\rangle \approx e^{i\varphi(t)} |n, \vec{R}(t)\rangle$$

provided that

$$\hbar \left| \langle m, \vec{R} | \frac{\partial H}{\partial t} | n, \vec{R} \rangle \right|$$

$$\ll (E_n - E_m)^2$$

for $n \neq m$.

Berry (1983):

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

what's the relative phase

between $|\psi(t=T)\rangle$

and $|\psi(t=0)\rangle$?

For many years, people

did not care about this

question, because

observable.

$$\langle \psi | \hat{A} | \psi \rangle$$

is independent of the phase of $|\psi\rangle$.

But, phases can be observable in interference.

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

Try a solution of the form

$$\boxed{|\psi(t)\rangle \equiv \equiv \underbrace{e^{-\frac{i}{\hbar}\int_0^t dt'\, E_n(\vec{R}(t'))}}_{\text{"dynamical phase"}} \underbrace{|\phi_n(t)\rangle}_{\left(\alpha\, |n, \vec{R}(t)\rangle\right)}}$$

(*)

$$e^{-\frac{i}{\hbar} E t} = e^{-\frac{i}{\hbar}\int_0^t E(t')\,dt'}$$

what is $|\phi_n(t)\rangle$?

Schrödinger eq:

$$i\hbar\,|\dot{\psi}(t)\rangle = \mathcal{H}(t)\,|\psi(t)\rangle$$

$$0 = \langle\psi(t)|\left(\mathcal{H}(t) - i\hbar\frac{\partial}{\partial t}\right)|\psi(t)\rangle$$

Using $(*)$,

$$\Rightarrow \boxed{0 = \langle\phi_n(t)|\dot{\phi}_n(t)\rangle}$$

Quantum version of the law of parallel transport!

$|\phi_n(t)\rangle$ is the analog of

the parallel-transported vector.

In analogy w/ the case of geometry, we express the parallel-transported state $|\phi_n(t)\rangle$ in terms of a fixed and single-valued orthonormal basis $\{|n, \vec{R}\rangle\}$:

$$\boxed{|\phi_n(t)\rangle \equiv e^{i\gamma_n(t)} |n, \vec{R}(t)\rangle} \quad (**)$$

(analog of

$$\vec{\phi}(t) = e^{i\theta(t)} \vec{u}(t)$$

in geometry)

$\gamma_n(t)$ is the analog of $\theta(t)$.

Plug $(**)$ in

$$\langle \phi_n(t) \,|\, \dot{\phi}_n(t) \rangle = 0$$

$$\Rightarrow \boxed{\begin{aligned} &\dot{\gamma}_n(t) = \\ &= i \langle n, \vec{R}(t) | \frac{d}{dt} | n, \vec{R}(t) \rangle \end{aligned}}$$

ex)

spin $\frac{1}{2}$ particle in a magnetic field:

$$\mathcal{H} = - g \mu_B \underbrace{\vec{S}}_{\uparrow} \cdot \vec{H}$$

spin $\frac{1}{2}$ operator.

$$\underbrace{|1; \vec{H}\rangle \; ; \; |2; \vec{H}\rangle}_{\text{eigenstates.}}$$

$$|1;\vec{H}\rangle \doteq \begin{pmatrix} \langle\uparrow|1;\vec{H}\rangle \\ \langle\downarrow|1;\vec{H}\rangle \end{pmatrix}$$

$$\langle 1;\vec{H}|\frac{d}{dt}|1;\vec{H}\rangle$$

$$= \left(\langle\uparrow|1;\vec{H}\rangle^*, \langle\downarrow|1;\vec{H}\rangle^*\right)$$

$$\begin{pmatrix} \frac{d}{dt}\langle\uparrow|1;\vec{H}\rangle \\ \frac{d}{dt}\langle\downarrow|1;\vec{H}\rangle \end{pmatrix}$$

Then,

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

where $\delta_n = -\frac{1}{\hbar}\int_0^T E_n(\vec{R}(t))\,dt$

= total dynamical phase

$$\boxed{\gamma_n} = i\int_0^T dt \,\langle n,\vec{R}|\frac{d}{dt}|n,\vec{R}\rangle$$

$$= \quad \uparrow \quad \frac{d}{dt} = \frac{d\vec{R}}{dt}\frac{d}{d\vec{R}}$$

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

= Berry phase.

"geometric phase"

$$\vec{R} = (R_1, R_2, R_3)$$