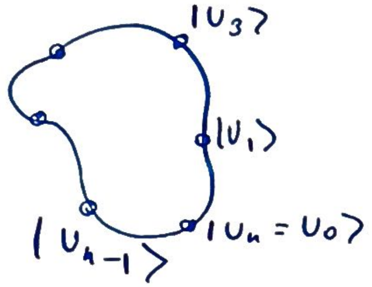
Based on lectures by D. Vanderbilt

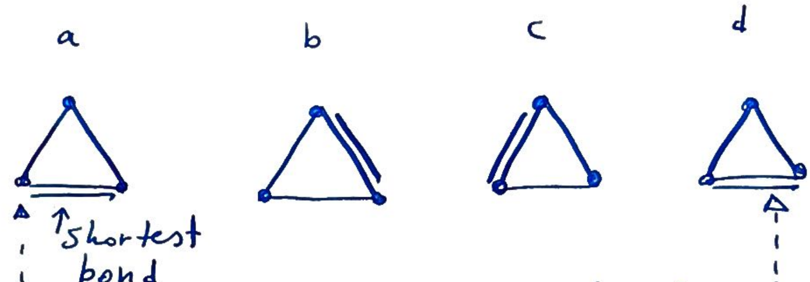
Lecture: **Q:** What is Berry phase (BP)? I

A: BP describes phase accumulation due to a motion of some complex vector around a close loop in the complex vector space.



DESCRETE VERSION

For a specific example, let's consider a triatomic molecule.



The BP is defined as

$$\boxed{\phi = -\mathrm{Im}\ln\left[\langle U_0|U_1\rangle\langle U_1|U_2\rangle \dots \langle U_{N-1}|U_0\rangle\right]}$$

For a complex vector $z = |z|e^{i\phi}$ $\quad \mathrm{Im}\ln z = \phi$.

Consider now our triatomic molecule

$$|U_a\rangle = |U_d\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad |U_b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\e^{2\pi i/3}\end{pmatrix} \quad |U_c\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\e^{4/3\pi i}\end{pmatrix}$$

then BP is given by:

$$\phi = -\mathrm{Im}\ln\left[\langle U_a|U_b\rangle\langle U_b|U_c\rangle\langle U_c|U_d\rangle\right] =$$
$$= -\mathrm{Im}\ln\left[\left(\frac{e^{\pi i/3}}{2}\right)^3\right] = -\pi.$$

At least mathematically the BP is independent of individual phases of $|u_j\rangle$. Let's introduce a new set of N states

$$|\tilde{U}_j\rangle = e^{-i\beta_j}|u_j\rangle \quad \leftarrow \beta_j \text{ is real}$$

We can show that in this case the BP is unaffected as $e^{\pm i\beta_j}$ along the path will cancel out.

So we should say that <u>BP is gauge invariant</u> and as such perhaps describes ~~on~~ some kind of Physics.

Continuous formulation of BP

In this formulation we ~~para~~ parametrize the path by a real variable λ such that $|u_\lambda\rangle$ traverses the path as λ evolves from 0 to 1, i.e. $|u_{\lambda=0}\rangle = |u_{\lambda=0}\rangle$ and $|u_\lambda\rangle$ is a smooth function of λ. Lets try to derive an expression similar to the descrete version.

$$\ln \langle u_\lambda | u_{\lambda+d\lambda}\rangle = \ln \langle u_\lambda | \left(|u_\lambda\rangle + d\lambda \frac{d|u\rangle}{d\lambda} + \dots \right)$$

$$= \ln\left(1 + d\lambda \langle u_\lambda | d_\lambda u_\lambda\rangle + \dots\right) = d\lambda \langle u_\lambda | \partial_\lambda u_\lambda \rangle + \dots \qquad \partial_\lambda \equiv \frac{d}{d\lambda}$$

Then BP is: $\boxed{\phi = -\mathrm{Im} \oint \langle u_\lambda | \partial_\lambda u_\lambda\rangle d\lambda}$

$$\mathrm{Re}\,\langle u_\lambda | \partial_\lambda u_\lambda\rangle = \langle u_\lambda | \partial_\lambda u_\lambda\rangle + \langle \partial_\lambda u_\lambda | u_\lambda\rangle = \partial_\lambda \langle u_\lambda | u_\lambda\rangle = 0$$

$\Downarrow$ $\langle u_\lambda | \partial_\lambda u_\lambda\rangle$ is pure imaginary and.

$$\boxed{\phi = \underbrace{\oint \langle u_\lambda | i\partial_\lambda u_\lambda\rangle d\lambda}}$$

Berry connection or Berry potential

$$A(\lambda) = \langle u_\lambda | i\partial_\lambda u_\lambda\rangle = -\mathrm{Im}\,\langle u_\lambda | \partial_\lambda u_\lambda\rangle$$

In terms of $A(\lambda)$:

$$\phi = \oint A(\lambda)\, d\lambda$$

Q: How Berry connection changes under gause transformation?

$|\tilde{u}_\lambda\rangle = e^{-i\beta(\lambda)}|u_\lambda\rangle$

$\uparrow$ real function

$\tilde{A}(\lambda) = \langle\tilde{u}_\lambda|\partial_\lambda \tilde{u}_\lambda\rangle = \langle u_\lambda| e^{i\beta(\lambda)}\, i\partial_\lambda\, e^{-i\beta(\lambda)}|u_\lambda\rangle =$

$= \langle u_\lambda|i\partial_\lambda|u_\lambda\rangle + \underbrace{\beta'(\lambda)}_{\frac{i\,\partial\beta}{\partial\lambda}}$

So BP is not gauge invariant! and it changes as:

$\tilde{A} = A + \frac{d\beta}{d\lambda}$. But what about BP?

$|\tilde{u}_{\lambda=1}\rangle = |\tilde{u}_{\lambda=0}\rangle \Rightarrow \beta_{\lambda=1} = \beta_{\lambda=0} + 2\pi m, \quad m = 0, 1 \ldots$

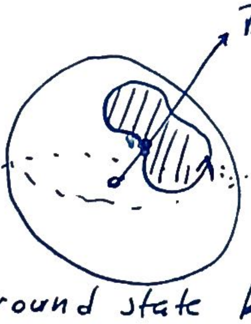
$\int_0^1 \frac{d\beta}{d\lambda} d\lambda = \beta_{\lambda=1} - \beta_{\lambda=0} = 2\pi m$ so for

$\tilde{\phi} = \oint \tilde{A}(\lambda)\, d\lambda = \underbrace{\oint \left(A\right.}_{=\phi} + \left.\frac{d\beta}{d\lambda}\right) d\lambda = \phi + 2\pi m$

So BP is still gauge invariant!

You can think of BP as the phase which still left over after moving in the loop.

EXAMPLE



let me illustrate this by considering a real physical problem.

imagine we have an eigenvector which is a ground state of some H_λ. We can smoothly evolve the ground state by changing λ, which in our case can be ~~#~~ magnetic B or electric fields E.

$\uparrow S$ a neutron at rest.

$H = -\gamma B \cdot \underbrace{S}_{= \hbar/2\, \sigma} = -\left(\frac{\gamma\hbar B}{2}\right)\hat{n}\cdot\sigma$

The ground state is independent of $|B|$ but depends on σ operator.

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So we can write instead $|U_n\rangle$ to emphasize that $|U\rangle$ depends on the direction of the magnetic field and not on its magnitude $|B|$.

Q: What's the BP of $|U_n\rangle$ as $\vec{n}$ carried around a loop in the magnetic field.

Lets try a simple descrete version:

① $\hat{n} \parallel \hat{z} \rightarrow$ rotate to $\hat{x} \rightarrow$ to $\hat{y} \rightarrow$ back to $\hat{z}$.

So we are tracing one octant of the sphere.

$$\phi = -\operatorname{Im} \ln \left[\langle \uparrow z | \uparrow x \rangle \langle \uparrow x | \uparrow y \rangle \langle \uparrow y | \uparrow z \rangle \right]$$

What we remember from QM 1 is that a spinor in arbitraty direction $\hat{n}$ is given by:

$$|\uparrow n\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2 \; e^{i\varphi} \end{pmatrix}$$

$|\uparrow x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ $\quad |\uparrow y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$ $\quad |\uparrow z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

Ignoring the normalization factors:

$$\phi = -\operatorname{Im} \ln \left[(1)(1+i)(1) \right] = -\pi/4$$

$\boxed{\text{Exersize:}}$ Show that for N spinors taking N equally spaced values from 0 to 2π gives:

a) $\phi = -N \tan^{-1} \left[\dfrac{\sin^2(\theta/2) \sin(2\pi/N)}{\cos^2(\theta/2) + \sin^2(\theta/2)\cos(2\pi/N)} \right]$

b) find $\phi(\theta)$ for $N \to \infty$

c) for $\theta = 45°$ compute numerically $N = 3, 4, 6, 12 \ldots 100$ and compare to $N \to \infty$

THE END of the easy version of Berry phase

Spin 1/2 B.P.

$$H = \bar{h} \cdot \bar{\sigma} = \sum_{i=1}^{3} h_i \sigma_i$$

h in polar E^3: $h = (h \sin\theta \cos\varphi,\ h \sin\theta \sin\varphi,\ h\cos\theta)$

The eigenstates with $\pm h$ are

$$|-\rangle = \begin{pmatrix} \sin\theta/2 \; e^{i\varphi} \\ -\cos\theta/2 \end{pmatrix} \qquad |+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \; e^{-i\varphi} \\ \sin\theta/2 \end{pmatrix}$$

You will get the last for the class homework about B.P. and $s = 1/2$.

$$H|\pm\rangle = \pm h|\pm\rangle \quad \text{and} \quad \langle \pm | \bar{\sigma} | \pm \rangle = \pm \frac{\bar{h}}{|h|}$$

Now let's observe that:

$|\pm\rangle$ depend olly on 2 parameters θ, φ and eigenvalues only on $|h|$ that forms the sphere S^2

Let's calculate the B..

$$A_\theta^- = \langle -| i\partial_\theta |-\rangle = 0$$

$$A_\varphi^- = \langle -| i\partial_\varphi |-\rangle = \sin^2\left(\frac{\theta}{2}\right)$$

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$$\omega^{-}_{\theta\varphi} = \partial_\theta A^{-}_\varphi - \partial_\varphi A^{-}_\theta = \frac{1}{2}\sin\theta$$

The B.P. through a small element s^2:

$$\omega^{-}_{\theta\varphi}\, d\theta\, d\varphi = \frac{1}{2}\sin\theta\, d\theta\, d\varphi = \frac{1}{2}\, d\Omega$$

This result tells us that the 'magnetic' field (B. curvature) is constant everywhere on the surface of a sphere in parameter space.

Berry curvature over the whole S^2 $= \int_S \omega^{-}_{\theta\varphi}\, d\theta\, d\varphi = \frac{1}{2}\underbrace{\int d\Omega}_{=4\pi}$
$= 2\pi$

and B.P of a loop on S^2:

$$\gamma_- = \frac{1}{2}\int_S d\Omega = \frac{1}{2}\Omega_s$$ of the solid angle

Interestingly, the result does not depend on the gauge, i.e.

$$|-\rangle \to |-\rangle e^{i\Theta_-(\theta,\varphi)}$$
$$|+\rangle \to |+\rangle e^{i\Theta_+(\theta,\varphi)}$$

arbitrary smooth functions of position in the space

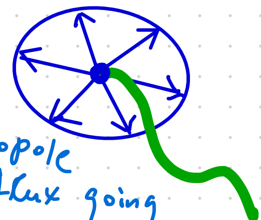
We can show that in general for a spin s we get:

$$\gamma_- = s \oint_S d\Omega = \mathbf{s}\, \Omega_s$$

$\uparrow$ spin

If we go back to the Cartesian coordinate parameter space of $\bar{h}$ the Berry curvature seen by the lower energy eigenstate $|-\rangle$ is:

$$\bar{b}_- = \mathbf{s} \frac{\bar{h}}{h^3}$$



Monopole flux going

semi infinite solenoid carrying a single quantum flux h/e

The total magnetic flux emanating from the sphere is h/e

We neglect the singular contribution from the infinitely thin solenoid

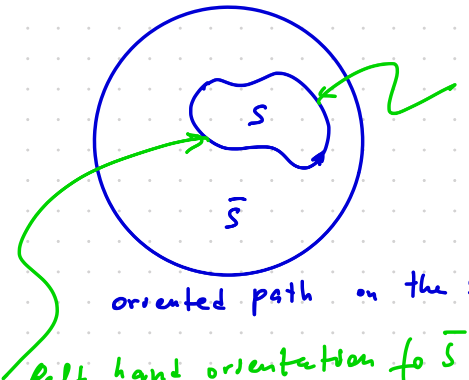
The Dirac monopole acts a point like magnetic charge.

Magnetic monopole with charge s located at the origin: b_- is equal $\mathbf{S} \times$ the local Gaussian curvature, and its direction is the local normal direction to the surface.

Also for $\epsilon_+ - \epsilon_- = 2|\vec{h}|$. = gap

Notice the gap vanishes at the origin (singularity)

Little imporant detail:



oriented path on the sphere S2

$\gamma_- = s\Omega_S$

$\bar{\gamma}_- = -s\,\Omega_{\bar{S}}$

we require both phases to be the same:

$\bar{\gamma}_-$ mod (2π)

Recall that total solid angle

$\Omega_S + \Omega_{\bar{S}} = 4\pi \Rightarrow$

$\gamma_- - \bar{\gamma}_- = s(4\pi) = 0 \mod (2\pi)$

as long as spin is $1/2 \cdot k$, k integer

Interesting idea: let's that spin is defined as $\gamma_- = s \oint_S d\Omega = s\,\Omega_S$ is lieu b/c. B. curvature in parameter space magnetic monopole $\Rightarrow$ topological argument for the quantization of spin is related to the Dirac argument for the quantization of the magnetic charge of monopoles.

The key is that Dirac string must be undetectable This can be the case if provided that flux inside the solenoid is an integer of hc/e, so the electron circling the solenoid will pick up the B. P. of $\pm 2\pi$ = $= 0$ phase shift = no string

Dirac argued that the reason an electric charge is quantized is because of the presence of magnetic monopoles.

'Magnetic monopoles' we 'detected' inside a solid state $Dy_2Ti_2O_7$ (read the posted paper on our web site)