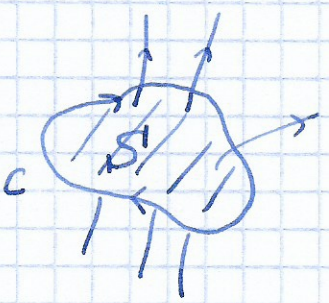
Interpretation

let $N=3$

magnetic flux



$$\Phi = \int_S \bar{B}\cdot d\bar{S} = \int_S (\bar{\nabla}\times\bar{A})\cdot d\bar{S} = \oint_C \bar{A}\cdot d\bar{r}$$

Stokes

$$\gamma_n = i\oint \underbrace{\langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle}_{\bar{A}} \cdot d\bar{R} = i\int_S \underbrace{\bar{\nabla}_{\bar{R}} \times \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle}_{\bar{B}}\, d\bar{S}$$

$$\bar{B} = i\,\bar{\nabla}_{\bar{R}} \times \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle$$

"magnetic field" in parameter space

γ_n – a flux in a parameter space

Is γ_n real?

$$0 = \bar{\nabla}_{\bar{R}} \underbrace{\langle \psi_n | \psi_n\rangle}_{=1} = \langle \bar{\nabla}_{\bar{R}}\psi_n | \psi_n\rangle + \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle =$$

$$= \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle^* + \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle = 0$$

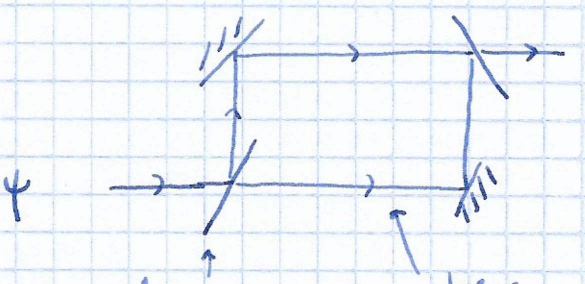
$$0 = (a+ib)^* + (a+ib) = 2a \rightarrow a = 0$$

$\langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle$ – pure imaginary

$$\gamma_n = i\oint \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n\rangle \cdot d\bar{R} \quad \text{– real} \qquad \square$$

Note, that if ψ_n is real $\gamma_n = 0$.

Is Berry phase measurable?



$$\psi = \frac{1}{\sqrt{2}}\psi_0 + \frac{1}{\sqrt{2}}\psi_0 e^{i\Gamma}$$

$$|\psi|^2 = \frac{1}{\sqrt{2}}\left(\psi_0 + \psi_0 e^{i\Gamma}\right)^* \frac{1}{\sqrt{2}}\left(\psi_0 + \psi_0 e^{i\Gamma}\right) = |\psi_0|^2(1+\cos\Gamma)$$

$$= |\psi_0|^2\, 2\cos^2(\Gamma/2)$$

any relative phase can be seen in interference measurement.

How does the adiabatic theorem enter?

The exact solution would be in a form

$$\psi_n(x,t) = \psi_n(x,t)e^{i\theta_n(t)}e^{i\gamma_n(t)} + \underbrace{\varepsilon\sum_{m\neq n} c_m(t)\,\psi_m(x,t)}_{\text{admixture of other states}}$$

$$\varepsilon = \frac{T_{int}}{T_{ext}}$$

$$i\hbar\left[\frac{\partial\psi_n}{\partial t}e^{i\theta_n}e^{i\gamma_n} \cancel{- \frac{i}{\hbar}E_n\psi_n e^{i\theta_n}e^{i\gamma_n}} + i\frac{d\gamma_n}{dt}\psi_n e^{i\theta_n}e^{i\gamma_n} + \right.$$

$$\left. + \varepsilon\sum_{m\neq n}\left(\frac{dc_m}{dt}\psi_m + c_m\frac{d\psi_m}{dt}\right)\right] =$$

$$= \cancel{E_n\psi_n e^{i\theta_n}e^{i\gamma_n}} + \varepsilon\sum_{m\neq n} E_m c_m \psi_m$$

$$\underbrace{\frac{\partial \psi_n}{\partial t} + i\frac{d\gamma_n}{dt}\psi_n}_{O(\varepsilon)} = -e^{-i\theta_n} e^{-i\gamma_n} \underbrace{\varepsilon \sum_{m\neq n} \underbrace{\left[\left(\frac{i}{\hbar} C_m E_m + \frac{dC_m}{dt}\right) + C_m \frac{\partial \psi_m}{\partial t}\right]}_{O(\varepsilon)}}_{O(\varepsilon^2)}$$

$\uparrow$ ε

(If the Hamiltonian didn't change $\frac{\partial \psi_n}{\partial t} = 0$ and $\frac{d\gamma_n}{dt} = 0$)

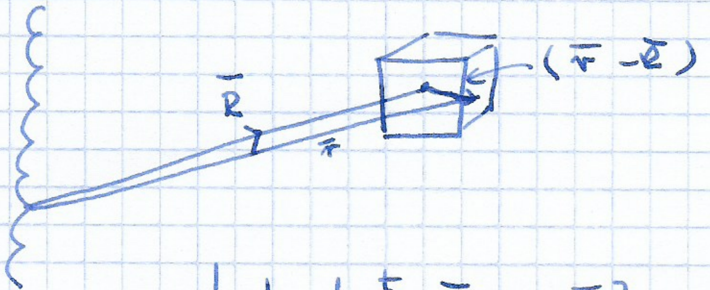
Note, formally eq. (*) on p. 76 should read

$$\frac{\partial \psi_n}{\partial t} + i\psi_n \frac{d\gamma_n}{dt} = -e^{-i\theta_n} \varepsilon \sum_{m\neq n} \left(\frac{i}{\hbar} C_m E_m + \frac{dC_m}{dt}\right)\psi_m$$

but $\int \psi_n^+ \, dx$ will eliminate the RHS.

§3. Aharonov - Bohm phase as a Berry phase

Let the charge be confined by a potential $V(\bar{r}-\bar{R})$



$\psi_n = \psi_n(\bar{r}, \bar{R})$

$$\left[\frac{1}{2m}\left[\frac{\hbar}{i}\bar{\nabla} - q\bar{A}\right] + V(\bar{r}-\bar{R})\right]\psi_n = E_n \psi_n$$

Solution is $\psi_n = e^{i\frac{q}{\hbar}\chi}\,\psi_n'$, $\chi = \int_{\bar{R}}^{\bar{r}} \bar{A}(\bar{r}')\cdot d\bar{r}'$

with $\left[-\frac{\hbar^2}{2m}\bar{\nabla}^2 + V(\bar{r}-\bar{R})\right]\psi_n' = E_n\psi_n'$ $(\bar{A}\to 0)$

$$\psi_n' = \psi_n'(\bar{r}-\bar{R})$$

Now we carry the "box" around the solenoid adiabatically

1) $\bar{\nabla}_{\bar{R}}\psi_n = \bar{\nabla}_{\bar{R}}\left[e^{i\frac{q}{\hbar}\chi}\psi_n'(\bar{r}-\bar{R})\right] =$

$$= -i\frac{q}{\hbar}\bar{A}(\bar{R})\,e^{i\frac{q}{\hbar}\chi}\psi_n'(\bar{r}-\bar{R}) + e^{i\frac{q}{\hbar}\chi}\bar{\nabla}_{\bar{R}}\psi_n'(\bar{r}-\bar{R})$$

2) $\langle\psi_n|\bar{\nabla}_{\bar{R}}\psi_n\rangle = \int d_3r\, e^{-i\frac{q}{\hbar}\chi}\psi_n'^*(\bar{r}-\bar{R})\,e^{i\frac{q}{\hbar}\chi}\left[-i\frac{q}{\hbar}\bar{A}(\bar{R})\psi_n'(\bar{r}-\bar{R}) + \right.$

$\left. + \bar{\nabla}_{\bar{R}}\psi_n'(\bar{r}-\bar{R})\right] =$

normalization

$$\overset{!}{=} -i\frac{q}{\hbar}\bar{A}(\bar{R}) - \underbrace{\int\left[\psi_n'(\bar{r}-\bar{R})\right]^*\underset{=\frac{i}{\hbar}\hat{p}}{\bar{\nabla}_{\bar{r}}}\psi_n'(\bar{r}-\bar{R})\,d_3r}_{\langle\hat{p}\rangle = 0 \text{ in a confined potential}} =$$

$\bar{\nabla}_{\bar{R}} = -\bar{\nabla}_{\bar{r}}$

$$= -i\frac{q}{\hbar}\bar{A}(\bar{R})$$

$$\boxed{\gamma_n = \frac{q}{\hbar}\oint \bar{A}(\bar{R})\cdot d\bar{R} = \frac{q}{\hbar}\int(\bar{\nabla}\times\bar{A})\cdot d\bar{S} = \frac{q}{\hbar}\Phi}.$$

§4. Emergent Berry monopole for a two-level system

We consider a zero-dimensional two-level system (TLS) with the Hamiltonian

$$\boxed{\hat{H} = \vec{d}\cdot\vec{\sigma} = \begin{pmatrix} d_z & d_x - i d_y \\ d_x + i d_y & -d_z \end{pmatrix}}$$

$$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

$$\vec{d} = (d_x, d_y, d_z)$$

E.g. $\vec{d} \leftrightarrow \vec{B}$ - external magnetic field → tutorials

Eigen problem

$$\boxed{\hat{H}\,|\psi_\pm\rangle = E_\pm\,|\psi_\pm\rangle}$$

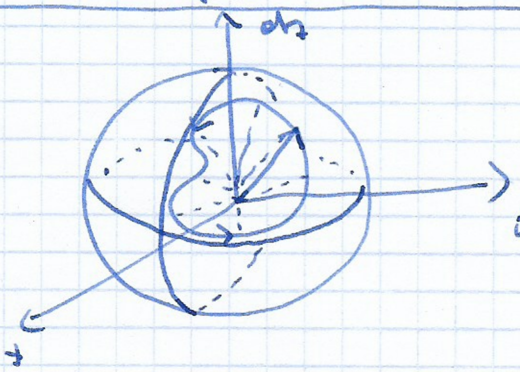
$$0 = \det\left[\hat{H} - E_\pm \mathbb{1}\right] = \begin{vmatrix} d_z - E_\pm & d_x - i d_y \\ d_x + i d_y & -d_z - E_\pm \end{vmatrix} =$$

$$= (d_z - E_\pm)(-d_z - E_\pm) - d_x^2 - d_y^2 =$$

$$= -d_z^2 \cancel{- d_z E_\pm} + \cancel{d_z E_\pm} + E_\pm^2 - d_x^2 - d_y^2 = 0$$

$$\boxed{E_\pm = \pm\sqrt{d_x^2 + d_y^2 + d_z^2} = \pm|\vec{d}|}$$

What will happen if we vary $\vec{d}$?



Bloch sphere — physics

Riemann sphere — mathematics

$$\begin{pmatrix} d_z - d & d_x - i d_y \\ d_x + i d_y & -d_z - d \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

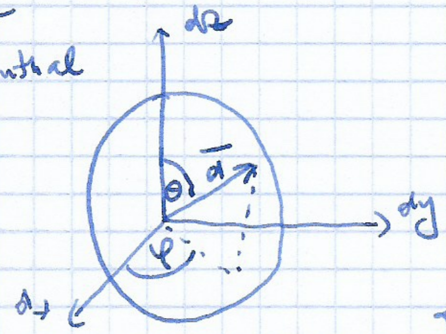
$E_+ = +d$

$|\psi_+\rangle = \begin{pmatrix} u \\ v \end{pmatrix}$

$$\begin{cases} (d_z - d)\,u + (d_x - i d_y)\,v = 0 \\ (d_x + i d_y)\,u - (d_z + d)\,v = 0 \quad \rightarrow \cancel{v = \frac{d_x + i d_y}{d_z + d}\,u} \end{cases}$$

we parametrize

θ-polar
φ-azimuthal



$d_x = d \sin\theta \cos\varphi$

$d_y = d \sin\theta \sin\varphi$

$d_z = d \cos\theta$

$$\begin{cases} (\cos\theta - 1)\,u + \sin\theta\,\overbrace{(\cos\varphi - i\sin\varphi)}^{e^{-i\varphi}}\,v = 0 \\ \sin\theta\,\underbrace{(\cos\varphi + i\sin\varphi)}_{e^{i\varphi}}\,u - (\cos\theta + 1)\,v = 0 \end{cases}$$

$$\boxed{\begin{aligned} \cos\theta &= 2\cos^2\tfrac{\theta}{2} - 1 = 1 - 2\sin^2\tfrac{\theta}{2} \\ \sin\theta &= 2\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2} \end{aligned}}$$

$$\begin{cases} -\cancel{2}\,\sin^{\cancel{2}}\tfrac{\theta}{2}\,u + \cancel{2}\,\cancel{\sin\tfrac{\theta}{2}}\cos\tfrac{\theta}{2}\,e^{-i\varphi}\,v = 0 \\ \cancel{2}\,\sin\theta/2\,\cancel{\cos\theta/2}\,e^{i\varphi}\,u - \cancel{2}\cos^{\cancel{2}}\tfrac{\theta}{2}\,v = 0 \end{cases}$$

$$\rightarrow \boxed{|\psi_+\rangle = \begin{pmatrix} \cos\frac{\theta}{2}\,e^{-i\varphi} \\ \sin\frac{\theta}{2} \end{pmatrix}}$$

similarly for $E_- = -d$

$$\boxed{|\psi_-\rangle = \begin{pmatrix} \sin\frac{\theta}{2}\,e^{-i\varphi} \\ -\cos\frac{\theta}{2} \end{pmatrix}}$$

when $\theta = \pi$ (south pole) $|\psi_-\rangle = \begin{pmatrix} e^{-i\varphi} \\ 0 \end{pmatrix}$ φ not defined at the south pole!

when $\theta = \pi$ (north pole) $|\psi\rangle = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$ is well defined

Indeed, the solution is given up to a global phase ($e^{i\varphi}$)

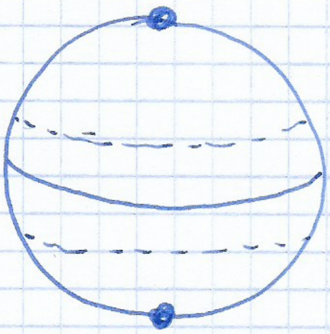
•) on the north hemisphere (pole)

$$\boxed{\begin{array}{ll} E_+ = +d & |\psi_+^{(n)}\rangle = \begin{pmatrix} \cos\frac{\theta}{2}\, e^{-i\varphi} \\ \sin\frac{\theta}{2} \end{pmatrix} \\[2em] E_- = -d & |\psi_-^{(n)}\rangle = \begin{pmatrix} \sin\frac{\theta}{2}\, e^{-i\varphi} \\ -\cos\frac{\theta}{2} \end{pmatrix} \end{array}}$$

•) on the south hemisphere (pole)

$$\boxed{\begin{array}{ll} E_+ = +d & |\psi_+^{(s)}\rangle = \begin{pmatrix} \cos\theta/2 \\ \sin\theta/2\, e^{i\varphi} \end{pmatrix} \\[2em] E_- = -d & |\psi_-^{(s)}\rangle = \begin{pmatrix} \sin\theta/2 \\ -e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix} \end{array}}$$

two gauges needed!



one cannot define a simple gauge without a singular point on S^2

→ similarity to a magnetic monopole

→ non zero Berry flux

→ the choice of a global phase is irrelevant for a time-independent problems

⇒ the time-dependent problem is more subtle

•) We consider a driven TLS - parameter dependent Hamiltonian $\theta = \theta(t)$, $\varphi = \varphi(t)$

$$\hat{H} = \hat{H}(\theta, \varphi)$$

We focus on the evolution of the ground state $\boxed{|\psi\rangle :\equiv |\psi_-\rangle}$ as (θ, φ) are varied adiabatically - the lowest level only / projection

$$E_-(\theta, \varphi) = -|\vec{d}(\theta, \varphi)| \neq 0$$

We compute the overlaps

$$\langle \psi(\theta, \varphi) | \psi(\theta + d\theta, \varphi) \rangle = \langle \psi(\theta, \varphi) | \psi(\theta, \varphi) \rangle + \langle \psi(\theta, \varphi) | \frac{\partial}{\partial \theta} \psi(\theta, \varphi) \rangle d\theta$$

$$\langle \psi(\theta, \varphi) | \psi(\theta, \varphi + d\varphi) \rangle = \langle \psi(\theta, \varphi) | \psi(\theta, \varphi) \rangle + \langle \psi(\theta, \varphi) | \frac{\partial}{\partial \varphi} \psi(\theta, \varphi) \rangle d\varphi$$

* * *

Remember Berry phase

$$\gamma_n = \oint_C \underbrace{i\langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n \rangle}_{\bar{A}} \cdot d\bar{R} = \int_S \underbrace{\bar{\nabla}_{\bar{R}} \times i\langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n \rangle}_{\bar{B} = \bar{\nabla}_{\bar{R}} \times \bar{A}} \cdot d\bar{S}$$

Berry vector potential (Berry connection)

Stokes

Berry field (curvature)

* * *

For TLS:

$$A_\theta = i\langle \psi | \partial_\theta \psi\rangle \quad , \quad A_\varphi = i\langle \psi | \partial_\varphi \psi\rangle$$

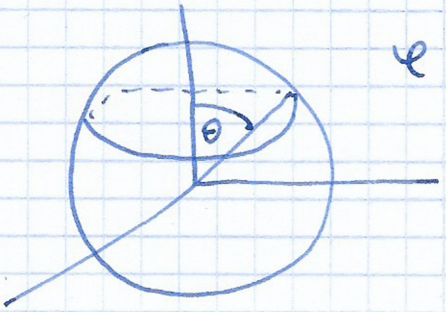
$$\partial_\theta |\psi_-^{(n)}\rangle = \begin{pmatrix} \frac{1}{2}\cos\frac{\theta}{2} e^{-i\varphi} \\ \frac{1}{2}\sin\frac{\theta}{2} \end{pmatrix} \qquad \partial_\varphi |\psi_-^{(n)}\rangle = \begin{pmatrix} -i\sin\frac{\theta}{2} e^{-i\varphi} \\ 0 \end{pmatrix}$$

$$\partial_\theta |\psi_-^{(s)}\rangle = \begin{pmatrix} -\frac{1}{2}\sin\frac{\theta}{2} \\ \frac{1}{2}\cos\theta/2\, e^{i\varphi} \end{pmatrix} \qquad \partial_\varphi |\psi_-^{(s)}\rangle = \begin{pmatrix} 0 \\ -i e^{i\varphi}\cos\theta/2 \end{pmatrix}$$

$$\boxed{\begin{matrix} A_\theta^{(n)} = 0 & , & A_\varphi^{(n)} = \sin^2\frac{\theta}{2} \\ A_\theta^{(s)} = 0 & , & A_\varphi^{(s)} = -\cos^2\theta/2 \end{matrix}}$$

Note: $A_\varphi^{(n)} - A_\varphi^{(s)} = 1 = \frac{\partial}{\partial\varphi}\underbrace{\varphi}_{\chi(\theta,\varphi)}$ – gauge transf.

Remarkably, the contour integral is gauge independent up to 2π factor



$\varphi \in (0, 2\pi)$

$$\Phi^{(n)} = \oint_{C_\theta} d\varphi\, A_\varphi^{(n)} = 2\pi\sin^2\frac{\theta}{2}$$

$$\Phi^{(s)} = \oint_{C_\theta} d\varphi\, A_\varphi^{(s)} = -2\pi\cos^2\theta/2$$

$$\boxed{\Phi^{(N)} - \Phi^{(S)} = 2\pi}$$

what is invariant is the Wilson loop

$$W(C_\theta) = e^{i\Phi^{(n)}} = e^{i\Phi^{(s)}}$$ (Baby version)

-> The Berry phase accumulated along a closed path is gauge invariant (up to 2π factor) and may be observable in interference experiments.

•) Berry field (curvature)

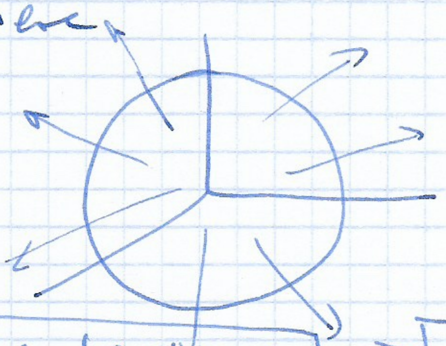
$$F_{\theta\varphi} = \partial_\theta A_\varphi - \partial_\varphi A_\theta = \frac{1}{2}\sin\theta$$ for (n) and (s) gauge independent

•) The total (Berry) flux

$$\Phi_{tot} = \iint_{S^2} d\varphi\, d\theta\, F_{\theta\varphi} = \frac{1}{2}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta = \boxed{2\pi}$$

-> can be viewed as an integral of $\frac{1}{2}\sin\theta$

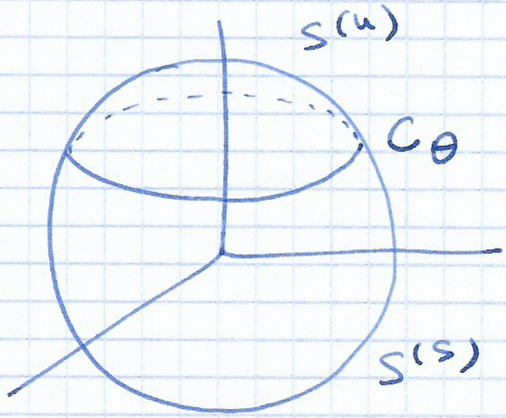
-> can be viewed as a flux of a radial field of constant length $\frac{1}{2}$ through a unit sphere



-> $\boxed{\text{topological feature}}$ -> $\boxed{\text{a monopole}}$

Th. the total Berry phase is always multiple of 2π

proof Take a two caps (n) and (s)



$$\iint_{S^2} d\theta\, d\varphi\, F_{\theta\varphi} \underset{\text{Stokes}}{=} \int_{C_\theta} d\varphi\, A^{(n)} - \int_{C_\theta} d\varphi\, A^{(s)}$$

$$\iint_{S^{(n)}} d\varphi\, d\theta\, F_{\theta\varphi} = \oint_{C_\theta} A^{(n)} d\varphi = 2\pi \sin^2\frac{\theta}{2}$$

$$\iint_{S^{(s)}} d\varphi\, d\theta\, F_{\theta\varphi} = -\oint_{C_\theta} A^{(s)} d\varphi = 2\pi \cos^2\frac{\theta}{2}$$

$$\Rightarrow \iint_{S^2} d\theta\, d\varphi\, F_{\theta\varphi} = 2\pi\left(\sin^2\frac{\theta}{2} + \cos^2\frac{\theta}{2}\right) = 2\pi$$

local gauge independent field

□

The total Berry flux does not depend on the shape of a closed contour C_θ and is quantized

$\rightarrow$ Chern number $\rightarrow$ topological invariant

o) Magnetic monopole interpretation

Let's go from the spherical angular parameters $(\theta, \varphi) \in S^2$ to the Euclidian space $\mathbb{R}^3$ spanned by (d_x, d_y, d_z).

$$\boxed{\bar{\nabla} = \hat{r}\frac{\partial}{\partial r} + \frac{1}{r}\hat{\theta}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}} \qquad \bar{A} = (A_\theta, A_\varphi)$$

$d = |\bar{d}| = \text{const.}$

$$\bar{\underset{\sim}{A}} = (\underset{\sim}{A}_x, \underset{\sim}{A}_y, \underset{\sim}{A}_z) = i\langle\psi|\bar{\nabla}_{\bar{d}}\psi\rangle =$$

$$= i\langle\psi|\left(\hat{\theta}\frac{1}{d}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{d\sin\theta}\frac{\partial}{\partial\varphi}\right)\psi\rangle$$

$$\boxed{\vec{\underset{\sim}{A}}^{(n)}} = i\left[\sin\frac{\theta}{2}e^{i\varphi}, -\cos\frac{\theta}{2}\right]\begin{bmatrix}\hat{\theta}\frac{1}{2d}\cos\frac{\theta}{2}e^{-i\varphi} + \hat{\varphi}\frac{1}{d\sin\theta}\left(-i\sin\frac{\theta}{2}e^{-i\varphi}\right) \\ \hat{\theta}\frac{1}{2d}\sin\frac{\theta}{2}\end{bmatrix} =$$

$$= i\left(\cancel{\frac{1}{2d}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\hat{\theta}} - \cancel{\frac{1}{2\theta}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\hat{\theta}} - i\frac{\sin^2\frac{\theta}{2}}{d\sin\theta}\hat{\varphi}\right) =$$

$$= \boxed{\frac{1-\cos\theta}{2d\sin\theta}\hat{\varphi}}$$ – regular at $\theta = 0$

$$\boxed{\vec{\underset{\sim}{A}}^{(s)} = -\frac{\cos^2\frac{\theta}{2}}{d\sin\theta}\hat{\varphi} = -\frac{1+\cos\theta}{2d\sin\theta}\hat{\varphi}}$$ – singular at $\theta = 0$

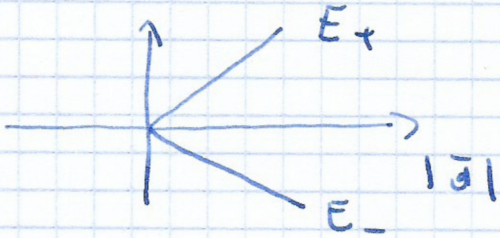
Po

Exact mapping onto a Dirac magnetic monopole

$\rho = \frac{1}{2}$ $n = 1$, $\hbar = 1$, $e = 1$, $d \to r$

The location of the Berry monopole at $\vec{d} = 0$ corresponds to a level degeneracy as

$E_{\pm} = \pm |\vec{d}| = 0$



The Berry field (curvature)

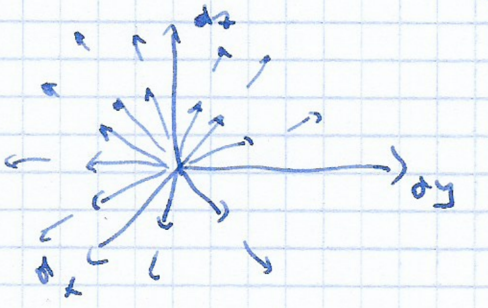
$$\boxed{\bar{\nabla} \times \bar{V} = \frac{1}{r \sin\theta}\left[\frac{\partial}{\partial\theta}\sin\theta\, V_\varphi - \frac{\partial V_\theta}{\partial\varphi}\right]\hat{r} + \dots}$$

$$\bar{F} = \bar{\nabla}_d \times \underset{\sim}{\bar{A}} =$$

$$= \frac{1}{d \sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \left(\frac{1-\cos\theta}{2d \sin\theta}\right)\right) = \frac{1}{2d^2}\,\hat{r}$$

$$\boxed{F = \frac{1}{2d^2}}$$

radial (in Bloch sphere) field



the same in $\underset{\sim}{\bar{A}}^{(N)}$ and $\underset{\sim}{\bar{A}}^{(S)}$ gauge

Berry flux $\oint \bar{F} \cdot d\bar{S} = \frac{4\pi d^2}{2d^2} = 2\pi$

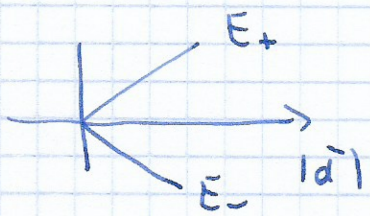
$$\boxed{\text{Berry (geometric) phase is related to a monopole in } (d_x, d_y, d_z) \text{ space}}$$

Why?

$\boxed{\text{TLS}} \xrightarrow[\text{evolution}]{\text{adiabatic}} \boxed{\text{Berry}}$

two spinor wave functions with no magnetic field

$|\psi_-\rangle$, $|\psi_+\rangle$



$|\psi_-^{IS,IN}\rangle$

One spinor wave function following an emergent gauge field (Berry potential) corresponding to a monopole in a parameter space

it accounts for the effect of virtual transitions to the excited state