Adiabatic Changes and Berry's Phase

Consider a physical system whose hamiltonian is an explicit *slow* function of time. By slow we mean ⓐ that either the rate of change is slow compared with the level spacing $/2\pi\hbar$ or ⓑ that the transitions to other states are negligible if the evolution is slow enough.

Examples: Ⓐ Molecules: the nuclei are heavy and their positions vary slowly on the scale of electron processes; Ⓑ a spin in a slowly varying magnetic field; Ⓒ many others.

Let $|\psi_n(t)\rangle$ be the *instantaneous* eigenstates of $\hat{H}(t)$, i.e.

$$H(t)\,|\psi_n(t)\rangle = E_n(t)\,|\psi_n(t)\rangle$$

$\{|\psi_n(t)\rangle\}$ are a basis at time t but it is a basis that ~~vary~~ changes with time (i.e. a moving frame).

If $|\psi(0)\rangle = |\psi_0(0)\rangle$ (for instance)

This does not imply that $|\psi(t)\rangle$, the evolved state $\left(|\psi(t)\rangle = T\, e^{-i\int_{t_0}^{t} H(t')\,dt'} |\psi(0)\rangle \right)$, is the instantaneous state $|\psi_0(t)\rangle$. This is true only for a time-independent system.

Furthermore, adiabatic evolution $\Rightarrow |\langle \psi_n(t) | \psi(t) \rangle| =$

$(n \neq 0)$

(i.e. no transitions to the new instantaneous excited states)

Still we expect $\underset{\substack{\uparrow \\ \text{evolved} \\ \text{state}}}{|\psi(t)\rangle} = e^{i\varphi(t)} \underset{\substack{\uparrow \\ \text{instantaneous} \\ \text{state}}}{|\psi_0(t)\rangle}$

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t)\, |\psi(t)\rangle$$

$$-\hbar \dot{\varphi}\, \cancel{e^{i\varphi}} |\psi_0\rangle + i\hbar \cancel{e^{i\varphi}} \frac{d}{dt} |\psi_0\rangle = E_0 \cancel{e^{i\varphi}} |\psi_0\rangle$$

Define $\frac{d}{dt} |\psi_0\rangle \equiv |\dot{\psi}_0\rangle = |\frac{d}{dt}\psi_0\rangle$

and write $\hbar\varphi = \hbar\gamma - \int_{t_0}^{t} dt'\, E_0(t')$

$$\hbar\dot{\varphi} = \hbar\dot{\gamma} - E_0$$

$$-\hbar\dot{\varphi} + i\hbar\langle\psi_0|\dot{\psi}_0\rangle = E_0$$

$$-\hbar\dot{\gamma} + \cancel{E_0} + i\hbar\langle\psi_0|\dot{\psi}_0\rangle = \cancel{E_0}$$

$$\Rightarrow \dot{\gamma} = i\langle\psi_0|\dot{\psi}_0\rangle$$

Is the phase γ physical? In many cases it is not since I can always redefine the wave function up to a phase

$$|\psi_0'(t)\rangle = e^{i\alpha(t)}|\psi_0(t)\rangle$$

$\Rightarrow \dot{\gamma}' = \dot{\gamma} - \dot{\alpha}$ and I can choose $\dot{\gamma}' = 0$

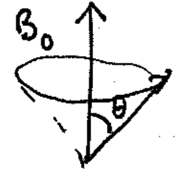
But there are cases in which one cannot do this!

<u>Example</u> : <u>Electron in a Precessing Magnetic Field</u>

There is a constant field $\vec{B} = B_0\hat{n}_z$ and

$$\vec{B}_1 = B_1(\hat{n}_x\cos\omega t + \hat{n}_y\sin\omega t)$$

$$\hbar\omega_0 = g\mu_B B_0 \;;\quad \hbar\omega_1 = g\mu_B B_1$$



$$\omega_0 = \bar{\omega}\cos\theta$$
$$\omega_1 = \bar{\omega}\sin\theta$$

$$\bar{\omega} = g\mu_B \bar{B} = \left(\sqrt{\omega_0^2+\omega_1^2}\right)\hbar \qquad (\hbar=1)$$

$\Rightarrow$ electron spin resonance.

At time t the magnetic field points along a direction with spherical coordinates

$(\theta,\phi) = (\theta, \omega t)$

$$\Rightarrow \quad H(\phi) = \frac{1}{2}\vec{B}(\phi)\cdot\vec{\sigma} \qquad (\hbar=1)$$

$$\vec{B}(\phi) = \omega_0\,\hat{n}_z + \omega_1(\cos\phi\,\hat{n}_x + \sin\phi\,\hat{n}_y)$$

$|\psi_\pm(t)\rangle$ are the instantaneous eigenstates

$$H(\phi)|\psi_\pm(\phi)\rangle = E_\pm(\phi)\,|\psi_\pm(\phi)\rangle$$

such that $|\psi_\pm(\phi+2\pi)\rangle = |\psi_\pm(\phi)\rangle$

$$|\psi_+(\phi)\rangle = \begin{pmatrix}\cos\theta/2\\ e^{i\phi}\sin\theta/2\end{pmatrix}$$

$\Rightarrow$

$$|\psi_-(\phi)\rangle = \begin{pmatrix}\sin\theta/2\\ -e^{i\phi}\cos\theta/2\end{pmatrix}$$

are the instantaneous eigenstates (polarized along the instantaneous $\vec{B}$)

If at $t_0=0$ $\quad |\psi(0)\rangle = |\psi_-(0)\rangle$ (antiparallel) ~~antiparallel~~

$\Rightarrow$

$$\Rightarrow |\psi(t)\rangle = i\frac{\omega}{\Omega}\sin\theta\,\sin\left(\frac{\Omega t}{2}\right)e^{-i\omega t/2}\,|\psi_+(t)\rangle$$

$$+\left[\cos\left(\frac{\Omega t}{2}\right) + i\left(\frac{\bar{\omega}-\omega\cos\theta}{\Omega}\right)\sin\frac{\Omega t}{2}\right]e^{+i\frac{\omega t}{2}}|\psi_-\rangle$$

$$\Omega = \sqrt{(\omega_0-\omega)^2+\omega_1^2} = \sqrt{\bar{\omega}^2+\omega^2-2\omega\bar{\omega}\cos\theta}$$

For $\omega \to 0$ (slow change) the probability to find the electron in the excited state $|\psi_+\rangle$ vanishes as ω^2 $\Rightarrow$ adiabatic limit.

For ω small, $\Omega \simeq \bar{\omega} - \omega\cos\theta$

$$\Rightarrow |\psi(t)\rangle \approx e^{i\frac{\Omega t}{2}}\,e^{-i\frac{\omega t}{2}}\,|\psi_-(t)\rangle$$

$$\approx e^{i\frac{\bar{\omega}t}{2}}\,e^{-i(\omega\cos\theta)\frac{t}{2}}\,e^{-i\frac{\omega t}{2}}\,|\psi_-(t)\rangle$$

$$+\,O\left(\frac{\omega}{\bar{\omega}}\right)$$

dynamical phase

$$E_-(t) = -\frac{\bar{\omega}}{2} \qquad (\hbar = 1)$$

$$e^{i\frac{\bar{\omega}t}{2}} = e^{-i\int_0^t dt'\,E_-(t')}$$

$\Rightarrow \gamma = -\frac{\omega t}{2}(\cos\theta + 1)$ = Berry's phase

$$\gamma\left(\frac{2\pi}{\omega}\right) = -\pi(\cos\theta + 1)$$

$\uparrow$
one period

Note $$\gamma\left(\frac{2\pi}{\omega}\right) = \int_0^{\frac{2\pi}{\omega}} i\,\langle\psi_-(\phi(t))|\,\dot{\psi}_-(\phi(t))\rangle\,dt$$

$$= \int_0^{\frac{2\pi}{\omega}} i\,\langle\psi_-(\phi(t))|\,\psi_-'(\phi(t))\rangle\,\frac{d\phi}{dt}\,dt$$

$$= \int_0^{2\pi} i\,\langle\psi_-(\phi)|\,\psi_-'(\phi)\rangle\,d\phi$$

$$|\psi_-(\phi)\rangle = \begin{pmatrix} \sin\theta/2 \\ -\cos\frac{\theta}{2}\,e^{i\phi}\end{pmatrix}$$

$$\frac{\partial}{\partial\phi}|\psi_-\rangle = |\psi_-'(\phi)\rangle = \begin{pmatrix} 0 \\ -i\cos\frac{\theta}{2}\,e^{i\phi}\end{pmatrix}$$

$$\langle\psi_-|\psi_-'\rangle = +i\cos^2\frac{\theta}{2}$$

$$i\langle\psi_-|\psi_-'\rangle = -\cos^2\frac{\theta}{2}$$

$$\cos^2\frac{\theta}{2} = \frac{1}{2}(1+\cos\theta)$$

$$\Rightarrow \gamma\left(\frac{2\pi}{\omega}\right) = \int_0^{2\pi/\omega} i\,\langle\psi_-|\dot{\psi}_-\rangle\,dt = -\pi(1+\cos\theta)$$

$\uparrow$
~~cycles~~
cycle!

Note: It is independent of $\phi(t)$!
(provided it is still adiabatic)

General Form of the Berry Phase

Let $H = H(\vec{R})$

$\hookrightarrow$ parameters (e.g. nuclear coords.)

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

(Born - Oppenheimer)

$t=0 \Rightarrow |\psi_0[\vec{R}(0)]\rangle$ and it evolves adiabatically

$$\Rightarrow |\psi(t)\rangle = e^{i\gamma(t)}\, e^{-i\int_0^t dt'\, E_0(\vec{R}(t'))\,dt'}\, |\psi_0(\vec{R}(t))\rangle$$

($\hbar = 1$)

$$|\vec{\nabla}\psi_0(\vec{e})\rangle \equiv \vec{\nabla}\,|\psi_0(\vec{R})\rangle \equiv \frac{\partial}{\partial\vec{R}}\,|\psi_0(\vec{R})\rangle$$

and $\vec{A}(\vec{R}) \equiv i\,\langle\psi_0(\vec{R}(t))|\vec{\nabla}\psi_0(\vec{R}(t))\rangle$

(which is <u>real</u>)

$$\Rightarrow \dot{\gamma} = i\,\langle\psi_0(t)|\dot{\psi}_0(t)\rangle$$

$$= i\,\langle\psi_0(\vec{R}(t))|\vec{\nabla}\psi_0(\vec{R}(t))\rangle \cdot \frac{d\vec{R}}{dt}$$

$$\equiv \vec{A}(\vec{R}(t)) \cdot \frac{d\vec{R}}{dt}$$

$$\Rightarrow \gamma(t) = \int_{\vec{R}(0)}^{\vec{R}(t)} \vec{A}(\vec{R}) \cdot d\vec{R}$$

For a closed path C in parameter space s.t.

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

$$\Rightarrow \gamma(T) = \oint_C \vec{A}(\vec{R}) \cdot d\vec{R} = \iint_\Sigma \underset{\text{Stokes!}}{\underset{\uparrow}{\vec{\nabla} \wedge \vec{A} \cdot d\vec{S}}}$$

$$C = \partial \Sigma$$

Clearly $|\psi_n(t)\rangle \to e^{i\underset{\text{twice differentiable!}}{\underset{\uparrow}{\lambda(\vec{R})}}} |\psi_n(R)\rangle$

$$\Rightarrow \vec{A}(R) \to \vec{A}(\vec{R}) - \vec{\nabla}\lambda$$

which does not change $\vec{\nabla} \wedge \vec{A}$

$\Rightarrow$ hence γ is "gauge invariant".

(i.e. it does not depend on the details of the adiabatic change)

How do we compute $\vec{\nabla} \wedge \vec{A}$?

$$(\vec{\nabla} \times \vec{A})_i = \varepsilon_{ijk} \nabla_j A_k$$

$$= \varepsilon_{ijk} \nabla_j (i \langle \psi_n(R) | \nabla_k \psi_n(R) \rangle)$$

$$= i \varepsilon_{ijk} \nabla_j \langle \psi_n(R) | \nabla_k \psi_n(R) \rangle$$

$$\equiv -\text{Im}\, \varepsilon_{ijk} \nabla_j \langle \psi_n | \nabla_k \psi_n(R) \rangle$$

which follows from

$$\langle \psi_n | \psi_n \rangle = 1 \Rightarrow \nabla_k \langle \psi_n | \psi_n \rangle = 0$$

$$\Rightarrow \mathrm{Re} \langle \psi_n | \nabla_k \psi_n \rangle = 0$$

$$\Rightarrow (\vec{\nabla} \wedge \vec{A})_i = - \mathrm{Im}\ \varepsilon_{ijk} \langle \nabla_j \psi_n | \nabla_k \psi_n \rangle$$

$$= - \mathrm{Im}\ \varepsilon_{ijk} \sum_{\ell} \langle \nabla_j \psi_n | \psi_\ell \rangle \langle \psi_\ell | \nabla_k \psi_n \rangle$$

For the case $n = \ell$ term vanishes (since $\langle \psi_n | \nabla_k \psi_n \rangle$ is imaginary)

$$\Rightarrow (\vec{\nabla} \wedge \vec{A})_i = - \mathrm{Im}\ \varepsilon_{ijk} \langle \nabla_j \psi_0 | \nabla_k \psi_0 \rangle \qquad \text{(for instance}$$

$$= - \mathrm{Im}\ \varepsilon_{ijk} \sum_{\ell \neq 0} \langle \nabla_j \psi_0 | \psi_\ell \rangle \langle \psi_\ell | \nabla_k \psi_0 \rangle$$

$$H(t)\, | \psi_n(t) \rangle = E_n(t)\, | \psi_n(t) \rangle$$

$$\Rightarrow \nabla_i H\, | \psi_n \rangle + H\, \nabla_i | \psi_n \rangle = \nabla_i E_n\, | \psi_n \rangle + E_n | \nabla_i \psi_n \rangle$$

$$\langle \psi_\ell | \nabla_i H | \psi_n \rangle + \langle \psi_\ell | H | \nabla_i \psi_n \rangle$$

$$= \nabla_i E_n \langle \psi_\ell | \psi_n \rangle + E_n \langle \psi_\ell | \nabla_i \psi_n \rangle$$

$$\Rightarrow \quad \langle \psi_l | \nabla_i \psi_n \rangle = \frac{\langle \psi_l | \nabla_i H | \psi_n \rangle}{E_n(R) - E_l(\vec{R})} \qquad (l \neq n)$$

$$\Rightarrow \quad (\vec{\nabla} \wedge \vec{A})_i = -\,\mathrm{Im} \sum_{l \neq 0} \frac{\langle \psi_0 | \vec{\nabla} H | \psi_l \rangle \wedge \langle \psi_l | \vec{\nabla} H | \psi_0 \rangle}{(E_l(0) - E_0(\vec{R}))^2}$$

Note: as we approach a degeneracy $(\vec{\nabla} \wedge \vec{A}) \to \infty$!

Back to spin resonance $(g=2)$

$$H = \mu_B \vec{B}(t) \cdot \vec{\sigma}$$

$$\vec{\nabla} H = \mu_B \vec{\sigma} \qquad (\text{i.e. } \vec{B}(t) \equiv \vec{R}(t))$$

$|\psi_0(\vec{B})\rangle$ is the state with spin $-\frac{1}{2}$ along $\vec{B}$

$$(\vec{\nabla} \wedge \vec{A})_i = -\,\mathrm{Im}\, \varepsilon_{ijk} \frac{\langle \psi_-(\vec{B}) | \nabla_j H | \psi_+(\vec{B}) \rangle \langle \psi_+(\vec{B}) | \nabla_k H | \psi_-(\vec{B}) \rangle}{(E_+(\vec{B}) - E_-(\vec{B})]^2}$$

$$E_+(\vec{B}) - E_-(\vec{B}) = 2\mu_B |\vec{B}|$$

If $\vec{B} = B\hat{n}_z \Rightarrow \quad \langle \psi_+ | \sigma_k | \psi_- \rangle = 0 \quad$ for $k=3$

$\Rightarrow (\vec{\nabla} \wedge \vec{A})_i = 0$ unless $i=3$

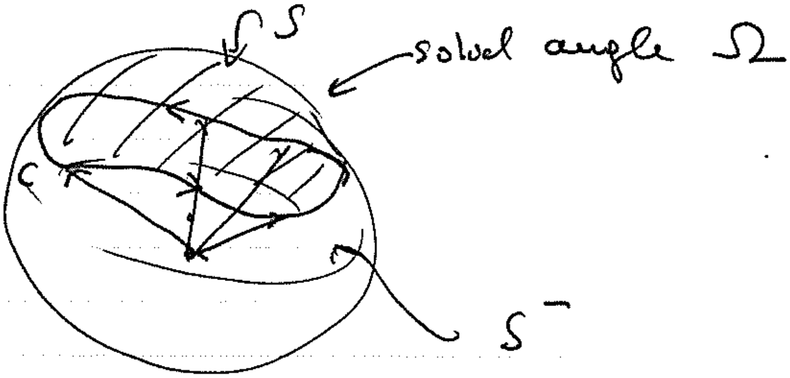
$$\langle \psi_+ | \sigma_1 | \psi_- \rangle = 1 \qquad \langle \psi_+ | \sigma_2 | \psi_- \rangle = -i$$

$$\Rightarrow \vec{\nabla} \wedge \vec{A}(B\hat{n}_z) = -\frac{1}{4B^2} \hat{n}_z \,\mathrm{Im}\Big[\langle \psi_+ | \sigma_1 | \psi_- \rangle^* \langle \psi_+ | \sigma_2 | \psi_- \rangle - \langle \psi_+ | \sigma_2 | \psi_- \rangle^* \langle \psi_+ | \sigma_1 | \psi_- \rangle \Big]$$

$$\Rightarrow \vec{\nabla} \wedge \vec{A} = -\frac{1}{2B^2}\hat{n}_z$$

In general $\boxed{\vec{\nabla} \times \vec{A} = -\frac{\hat{B}}{2|B|^2}}$ "magnetic monopole"

$$\int_C \vec{A} \cdot d\vec{B} = \iint_S \vec{\nabla} \times \vec{A} \cdot d\vec{s} = \pm \frac{\Omega}{2}$$ (Solid angle)



Ambiguity: which surface, the upper cap S^+ or the lower cap S^-. The phase ambiguity is

$$\gamma^+ - \gamma^- = \underset{\uparrow \text{ spin } 1/2\,!}{\frac{1}{2}}\, 4\pi = 2\pi$$

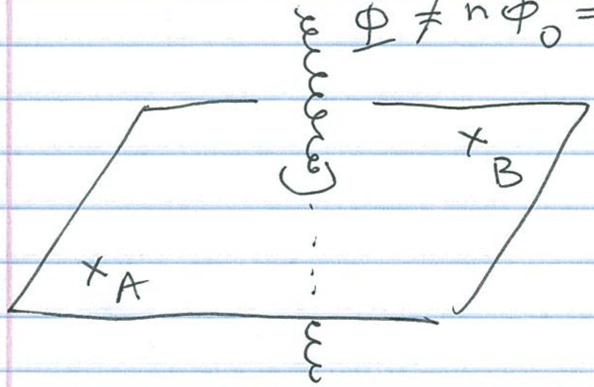
$\Rightarrow$ no physical effect since the spin is correctly quantized!

Berry Phase and the Aharonov-Bohm Effect

In Physics 580 we discuss the path integral picture of QM. We will now use it for the problem of a charged particle in 2D with a magnetic field concentrated at the origin.

$$\Phi \neq n\phi_0 = n\frac{hc}{e} = 2\pi n\frac{\hbar c}{e}$$

$$n \in \mathbb{Z}$$



Since we are threading flux at the origin we will assume that the particle cannot get to the flux tube.

The Lagrangian is

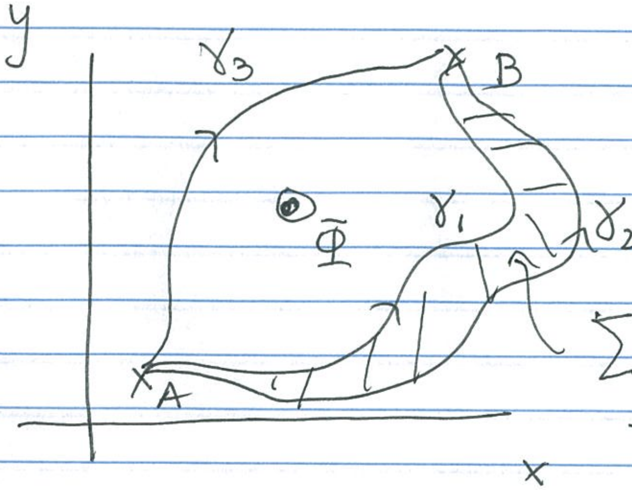
$$L = \frac{M}{2}\vec{v}^2 + \frac{e}{c}\vec{A}(\vec{r})\cdot\vec{v}$$

and the action is

$$S = \int_0^T dt\left[\frac{M}{2}\vec{v}^2 + \underset{\substack{\uparrow \\ \text{``Berry phase''}}}{\frac{e}{c}\vec{A}(\vec{r})\cdot\frac{d\vec{r}}{dt}}\right]$$

AB2

The path-integral is a sum over histories and sums over all of them. Suppose the initial state has the particle @ A and the final state @ B



$\vec{B} = \vec{\nabla}\times\vec{A} = \delta^2(\vec{r}-\vec{r}_0)\ \Phi$

Consider the paths γ_1 and γ_2

$$S[\gamma_1] = \int_0^T dt\ \frac{M}{2}\left(\frac{d\vec{r}}{dt}\right)^2 + \frac{e}{c}\int_{\gamma_1} d\vec{r}\cdot\vec{A}(\vec{r}(t))$$

and $$S[\gamma_2] = \int_0^T dt\ \frac{M}{2}\left(\frac{d\vec{r}}{dt}\right)^2 + \frac{e}{c}\int_{\gamma_2} d\vec{r}\cdot\vec{A}(\vec{r}(t))$$

$$\int_{\gamma_1} d\vec{r}\cdot\vec{A}(\vec{r}(t)) - \int_{\gamma_2} d\vec{r}\cdot\vec{A}(\vec{r}(t)) =$$

$$= \oint_{\gamma_1^+\cup\gamma_2^-} d\vec{r}\cdot\vec{A}(\vec{r}(t))$$

since $\oint_\gamma d\vec{r} \cdot \vec{A}(\vec{r}) = \iint_\Sigma d\vec{s} \cdot \vec{\nabla} \times \vec{A}$

$$= \iint_\Sigma d\vec{s} \cdot \vec{B}$$

But $\vec{B} = 0$! inside $\gamma = \gamma_1^+ \cup \gamma_2^-$

$\Rightarrow$ The weight of the two paths has the same phase factor

$$e^{i \frac{e}{c\hbar} \int_{\gamma_1} d\vec{r} \cdot \vec{A}(\vec{r})} = e^{i \frac{e}{\hbar c} \int_{\gamma_2} d\vec{r} \cdot \vec{A}(r)}$$

What about γ_3? Now $\int_A^B d\vec{r} \cdot \vec{A}(r)\Big|_{\gamma_1} \neq$

$$\int_A^B dr \cdot \vec{A}(\vec{r})\Big|_{\gamma_3}$$

since $\oint_{\bar{\gamma} = \gamma_1^+ \cup \gamma_3^-} d\vec{r} \cdot \vec{A} \equiv \iint_{\Sigma'} d\vec{s} \cdot \vec{B} = \Phi$

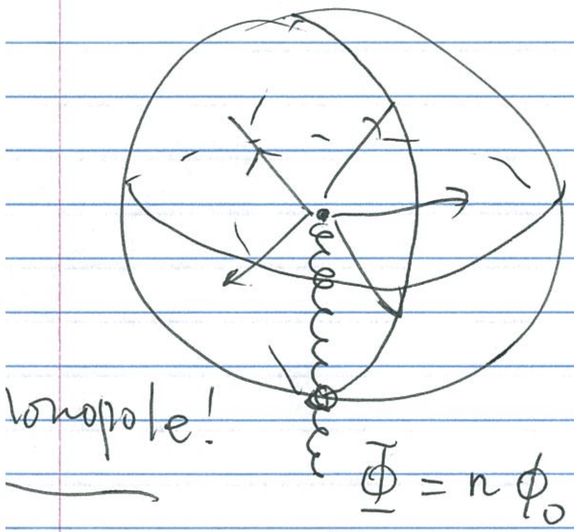
$$\Rightarrow \cancel{e^{i\gamma_1}} \; e^{\frac{ie}{\hbar c}\int_{\gamma_1} A \cdot dr} \; e^{-\frac{ie}{\hbar c}\int_{\gamma_2} \vec{A} \cdot \vec{r}} = e^{i \frac{e}{\hbar c} \Phi}$$

Interference! $\phi_0 = \frac{hc}{e} = 2\pi \frac{\hbar c}{}) = e^{i \frac{\Phi}{\phi_0} 2\pi}$

⇒ The flux tube is <u>invisible</u> if $\Phi = n\phi_0$ but <u>not</u> if $\Phi \neq n\phi_0$

Notice that the particle always is in places with $\vec{B} = 0$!

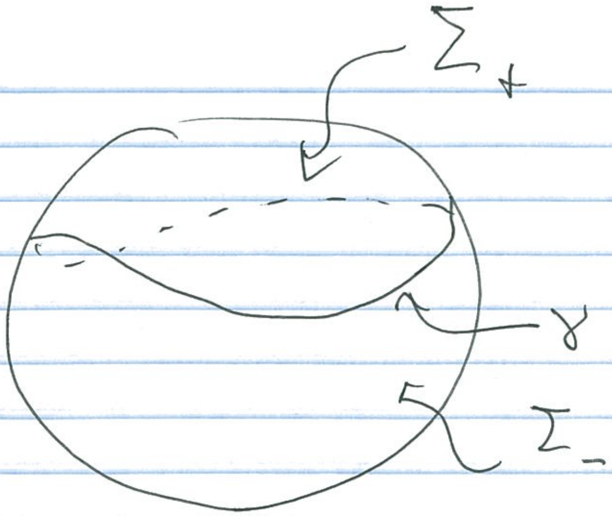
Charged particle on a sphere



$|\vec{r}| = R$ fixed

$$S = \int_0^T dt \, \frac{M}{2}\left(\frac{d\vec{r}}{dt}\right)^2 + \frac{e}{c}\oint_0^T dt \, \frac{d\vec{r}}{dt} \cdot \underset{\underset{\text{monopole!}}{\uparrow}}{\vec{A}(\vec{r})}$$

AB5



$$\int_0^T dt\ \vec{A}(\vec{r}(t))\cdot\frac{d\vec{r}}{dt} = \oint_\gamma d\vec{r}\cdot\vec{A}(\vec{r}(t))$$

$$= \oiint_{\Sigma^+} d\vec{s}\cdot\vec{B}(\vec{r}) = -\iint_{\Sigma^-} d\vec{s}\cdot\vec{B}(\vec{r})$$

Total ambiguity $\iint_{\Sigma^+} + \iint_{\Sigma^-} =$

$$= B\,4\pi R^2 = \text{flux}$$

B