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: ~~[illegible]~~ the nuclei are heavy and their ~~[illegible]~~ 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 $\Rightarrow |\langle \psi_n(t)|\psi(t)\rangle| = 0$ $(n \neq 0)$

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

Still we expect $|\psi(t)\rangle = e^{i\varphi(t)}\, |\psi_0(t)\rangle$

evolved state   instantaneous state

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

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

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 $\dot{\gamma}' = 0$

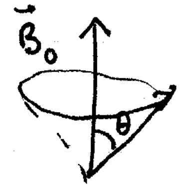
But there are cases in which one cannot do this!

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

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

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

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



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

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

$\Rightarrow$ electron spin resonance.

At time t the ~~E~~ 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)~~

$\Rightarrow$

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

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

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

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, $\Omega\simeq\bar\omega-\omega\cos\theta$

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

$$\approx \underbrace{e^{i\frac{\bar\omega t}{2}}}_{\text{dynamical phase}}e^{-i(\omega\cos\theta)\frac{t}{2}}e^{-i\frac{\omega t}{2}}|\psi_-(t)\rangle + O\left(\frac{\omega}{\bar\omega}\right)$$

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

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

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

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

one period

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

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

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

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

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

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

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

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

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

~~cycle~~ Cycle!

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

General Form of the Berry Phase

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

↳ 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

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

$(\hbar = 1)$

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

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.

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

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

$$C = \partial \Sigma$$

Stokes!

Clearly $\quad |\psi_n(t)\rangle \to e^{i\lambda(\vec{R})} \, |\psi_n(R)\rangle$

twice differentiable!

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

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 <u>adiabatic</u> change)

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

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

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

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

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

which follows from

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

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

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

$$= - \mathrm{Im} \; \varepsilon_{ijk} \sum_l \langle \nabla_j \psi_n | \psi_l \rangle \langle \psi_l | \nabla_k \psi_n \rangle$$

For the case $n=0$, the $l=0$ term vanishes

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

$$= - \mathrm{Im} \; \varepsilon_{ijk} \sum_{l \neq 0} \langle \nabla_j \psi_0 | \psi_l \rangle \langle \psi_l | \nabla_k \psi_0 \rangle$$

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

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

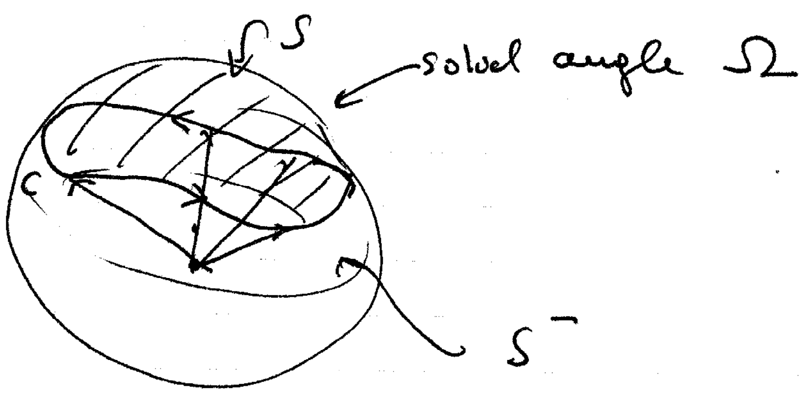
$$\langle \psi_l | \nabla_i H | \psi_n \rangle + \langle \psi_l | H | \nabla_i \psi_n \rangle$$

$$= \nabla_i E_n \langle \psi_l | \psi_n \rangle + E_n \langle \psi_l | \nabla_i \psi_n \rangle$$

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

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

$$\gamma^+ - \gamma^- = \frac{1}{2} 4\pi = 2\pi$$

↑ spin $1/2$!

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