Adiabatic Approximation

Let's assume that our Hamiltonian depends on a certain parameter s and

$$H[s]\,|n[s]\rangle = E_n[s]\,|n[s]\rangle$$

$$\langle m[s]|n[s]\rangle = \delta_{mn}$$

Thus, we can define eigenstates and eigen energies for any value of s.

Now let's consider the situation when $s = s(t)$. Obviously, we can now identify the eigenstates and energies for any moment of time, but this basis will be changing in time.
Slow change in s means small variation in states, but the change after a longer time evolution can be significant.

Now we need to solve the time-dependent Schrodinger equation

$$i\hbar \frac{\partial \alpha(t)}{\partial t} = \hat{H}[s(t)]\,\alpha(t)$$

As usual, we are going to decompose the state in the basis of eigenfunctions

$$|\alpha(t)\rangle = \sum_n C_n(t)\, e^{i\theta_n(t)}\, |n[s(t)]\rangle$$

comparing this with the time-independent $\hat{H}$ case

$$|\alpha(t)\rangle = \sum_n c_n\, e^{-i\frac{E_n t}{\hbar}}\, |n\rangle$$

and writing for smal Δt $\theta_n(\Delta t) \approx -\frac{iE_n \Delta t}{\hbar}$,

we can find that

$$\theta_n(t) = -\frac{i}{\hbar}\int_0^t E_n[s(t')]\,dt' \qquad \dot{\theta}_n = -\frac{iE_n}{\hbar}$$

$$i\hbar\frac{\partial|\alpha\rangle}{\partial t} = i\hbar\sum_n\Big[\dot{c}_n e^{i\theta_n}|n[s(t)]\rangle + \cancel{c_n e^{i\theta_n}(i\dot{\theta}_n)|n[s(t)]\rangle} + c_n e^{i\theta_n}\frac{\partial}{\partial t}|n\rangle\Big]$$

$$= \hat{H}|\alpha\rangle = \cancel{\sum_n c_n e^{i\theta_n}} E_n|n\rangle$$

$$i\hbar\sum_n\Big\{\dot{c}_n e^{i\theta_n}|n\rangle + c_n e^{i\theta_n}\frac{\partial}{\partial t}|n[s(t)]\rangle\Big\} = 0$$

$$i\hbar\,\dot{c}_m e^{i\theta_m} = -\sum_n c_n e^{i\theta_n}\langle m|\frac{\partial}{\partial t}|n[s(t)]\rangle$$

$$\dot{c}_m = -\sum_n c_n e^{i(\theta_n-\theta_m)}\langle m|\frac{\partial}{\partial t}|n[s(t)]\rangle$$

At the same time

$$H[s(t)]\,|n[s(t)]\rangle = E_n[s(t)]\cdot|n[s(t)]\rangle$$

$$\frac{\partial H}{\partial t}|n\rangle + H\frac{\partial|n\rangle}{\partial t} = \frac{\partial E_n}{\partial t}|n\rangle + E_n\frac{\partial|n\rangle}{\partial t}$$

$$\langle m|\frac{\partial H}{\partial t}|n\rangle + E_m\langle m|\frac{\partial|n\rangle}{\partial t} = \frac{\partial E_n}{\partial t}\delta_{nm} + E_n\langle m|\frac{\partial|n\rangle}{\partial t}$$

for $m \neq n$ — for $m = n$

$$\langle m|\frac{\partial|n\rangle}{\partial t} = \frac{1}{E_n - E_m}\langle m|\dot{H}|n\rangle; \qquad \langle m|\frac{\partial H}{\partial t}|m\rangle = \frac{\partial E_m}{\partial t}$$

or, more precisely

$$\langle m|\frac{\partial}{\partial t}|n[s(t)]\rangle = \frac{1}{E_n - E_m}\langle m|\dot{H}[s(t)]|n\rangle$$

$$\dot{c}_m = \underbrace{- c_m \langle m | \frac{\partial}{\partial t} | m\rangle}_{\text{evolution of the same state}} - \underbrace{\sum_{n\neq m} c_n e^{i(\theta_n - \theta_m)} \frac{\langle m|\dot{H}|n\rangle}{E_n - E_m}}_{\text{transitions b/w state}}$$

Adiabatic approximation $\longrightarrow$ we assume that the system stays in the same quantum state $|m[s(t)]\rangle$ as time progresses. That means the second term is negliggeable.

$$\left|\langle m|\frac{\partial m\rangle}{\partial t}\right| \sim \frac{E_m}{\hbar} \quad ; \langle m|\dot{H}|m\rangle \sim \frac{\partial E_m}{\partial t} \sim \frac{E_m}{\tau}$$

So in order for the first term to dominate

$$\frac{E_m}{\hbar} \gg \frac{E_m}{\tau(E_m - E_n)} \sim \frac{1}{\tau}$$

τ - characteristic time-scale for $s(t)$ change

Adiabatic apporoximation $\Rightarrow$

$\tau \gg \hbar/E_m$ slow variation

Then

$$\dot{c}_m = - c_m \langle m|\frac{\partial}{\partial t}|m\rangle$$

$$c_m = c_m(s_0)\, e^{-\int_0^t \langle m|\frac{\partial}{\partial t'}|m\rangle dt'} = c_m(s_0)\, e^{i\gamma_m(t)}$$

$s_0 = s[t=0]$

$$\gamma_m = i\int_0^t \langle m[s(t')]|\frac{\partial}{\partial t'}|m[s(t')]\rangle dt'$$

γ_m is real

$$\frac{\partial}{\partial t}\langle m|m\rangle = \left[\frac{\partial}{\partial t}\langle m|\right]|m\rangle + \langle m|\left[\frac{\partial}{\partial t}|m\rangle\right] = 0$$

$$\langle m|\frac{\partial |m\rangle}{\partial t} = -\frac{\partial\langle m|}{\partial t}|m\rangle = -\left(\langle m|\frac{\partial |m\rangle}{\partial t}\right)^*$$

purely imaginary

So if we start at one of the eigenstates at $t=0$

$$|\alpha(t=0)\rangle = |n\rangle \qquad c_n = 1, \; C_m = 0 \quad m \neq n$$

then $|\alpha(t)\rangle = e^{i\gamma_n} e^{i\theta_n} |n[s(t)]\rangle$

if $s(t) = s_0$ no time dependence

$$\gamma_n = i\int_0^t \langle n|\frac{\partial}{\partial t}|n\rangle\, dt = i\int_0^t \left(-\frac{iE_n}{\hbar}\right) dt = \frac{E_n t}{\hbar}$$

$$\theta_n = -\frac{iE_n t}{\hbar}$$

and $|\alpha(t)\rangle = |n\rangle$

So in adiabatic approximation the only consequence of time variation of the parameters is an extra phase factor $e^{i\gamma_n}$. But the phase of the wave function does not matter, right?!

Berry's Phase

$$\gamma_n = i\int_0^t \langle n|\frac{\partial}{\partial t}|n[s(t)]\rangle\, dt$$

$$\frac{\partial}{\partial t}|n[s(t)]\rangle = \sum_i \frac{\partial|n\rangle}{\partial s_i}\frac{\partial s_i}{\partial t}$$

where s_i are dimentions of the parameter s

s = 3D vector $\vec{s} = \{s_1, s_2, s_3\}$

Example: s is $\vec{r}$

$$\frac{\partial}{\partial t}|n(\vec{r}(t))\rangle = \frac{\partial|n\rangle}{\partial x}\underbrace{\frac{\partial x}{\partial t}}_{v_x} + \frac{\partial|n\rangle}{\partial y}\underbrace{\frac{\partial y}{\partial t}}_{v_y} + \frac{\partial|n\rangle}{\partial z}\underbrace{\frac{\partial z}{\partial t}}_{v_z}$$

$$\int_0^t \langle n|\frac{\partial}{\partial t}|n(\vec{r}(t))\rangle dt = \int_0^t \langle n|(\nabla|n(\vec{r})\rangle)\, \underbrace{\vec{v}\,dt}_{d\vec{r}} = \int_{C(t)} \langle n|(\nabla n(\vec{r})\rangle)\, d\vec{r}$$

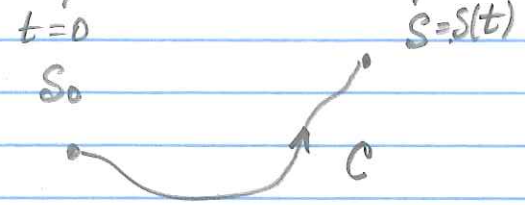
$C(t)$ line integral along the trajectory

Obviously, we can generalize this for any s-space, defining $\nabla_s \to \sum_i \frac{\partial}{\partial s_i} \vec{e}_{s_i}$

Then

$$\gamma_n = i \int_{C(t)} \langle n[\vec{s}] | \nabla_s | n[\vec{s}] \rangle \, d\vec{s}$$

The value of the phase does not depend on time, but rather on the "path" of the system in s-parameter space



Coming back to the question - should we worry about this phase?
If we can get rid of it by renormalizing the state

$$|\tilde{n}[s]\rangle = e^{i\alpha_n[s]} |n[s]\rangle$$

such that $\tilde{\gamma}_n(t) = \gamma_n(t) + \alpha_n[s_0] - \alpha_n[s(t)]$
If we can find such α_n, then $\{|\tilde{n}[s]\rangle\}$ and $\{|n[s]\rangle\}$ are equivalent

For this to happen $\gamma_n(t) = 0$ for $S[t] = S_0$ $\forall t$
or

$$\oint_C \langle n[s] | \nabla_s | n[\vec{s}] \rangle \, d\vec{s} = 0$$

This also means $\gamma_n(t)$ does not depend of the path $C(t)$.

What if $\gamma_n(t)$ over closed path is not zero?

Stokes theorem

$$\gamma_n(t) = i \oint_C \langle n | \nabla_{\vec{s}} | n \rangle \, d\vec{s} = i \int_{A_C} \nabla_{\vec{s}} \times \left(\langle n | \nabla_{\vec{s}} | n \rangle \right) d\vec{a}_{\vec{s}}$$

A - an area in $\vec{s}$ - space, enclosed by C

$da_{\vec{s}}$ - area element

$$\nabla_{\vec{s}} \times \left(\langle n | \nabla_{\vec{s}} | n \rangle \right) = \left(\nabla_{\vec{s}} \langle n | \right) \times \left(\nabla_{\vec{s}} | n \rangle \right) = \sum_m \left[\nabla_{\vec{s}} \langle n | \right] | m \rangle \times$$

$$\times \langle m | \left[\nabla_{\vec{s}} | n \rangle \right]$$

$$\nabla_{\vec{s}} \left(H[s] | n[s] \rangle = E_n[s] \, | n[s] \rangle \right.$$

$$\left(\nabla_{\vec{s}} H \right) \cdot | n \rangle + H \nabla_{\vec{s}} | n \rangle = \left(\nabla_{\vec{s}} E_n \right) | n \rangle + E_n \left(\nabla_{\vec{s}} | n \rangle \right)$$

for $n \neq m$

$$\langle m | \nabla_{\vec{s}} H | n \rangle + E_m \langle m | \nabla_{\vec{s}} | n \rangle = E_n \langle m | \left[\nabla_{\vec{s}} | n \rangle \right]$$

$$\langle m | \left[\nabla_{\vec{s}} | n \rangle \right] = \frac{\langle m | \nabla_{\vec{s}} H | n \rangle}{E_n - E_m}$$

what about $n = m$?

$$\nabla_{\vec{s}} \langle n | n \rangle = \underbrace{\left[\nabla_s \langle n | \right] | n \rangle}_{\vec{A}} + \underbrace{\langle n | \left[\nabla_{\vec{s}} | n \rangle \right]}_{-\vec{A}} = 0$$

thus $\left[\nabla_s \langle n | \right] | n \rangle \times \langle n | \left[\nabla_{\vec{s}} | n \rangle \right] = 0$

Thus

$$\gamma_n[C] = i \int_{A_C} \underbrace{\left\{ \sum_{m \neq n} \frac{\langle n | \nabla_{\vec{s}} H | m \rangle \langle m | \nabla_{\vec{s}} H | n \rangle}{(E_n - E_m)^2} \right\}}_{\vec{B}_n[s]} d\vec{a}_{\vec{s}}$$

Berry phase is the flux of the vector $\vec{B}$ through a surface enclosed by the contour C.

Example: a particle with non-zero angular momentum in a slowly varying magnetic field

Our time-varying parameter $\vec{B} = \vec{B}(t)$

$$\hat{H}[\vec{B}] = \mu \vec{B} \vec{J} + \hat{H}_0$$

μ – a constant relating magnetic and angular moment

For any moment of time we direct z-axis along $\vec{B}$; $\vec{B} = B_0 \vec{e}_z(t)$

$$\hat{H}[\vec{B}] = \mu B_z J_z (+ H_0)$$ additional $\hat{H}$ terms, independent of $\vec{J}$

$$\hat{H}\,|m[\vec{B}]\rangle = \mu \vec{B}\vec{J}\,|m\rangle = \mu B_z J_z\,|m\rangle = \hbar \mu B_0 m\,|m\rangle$$

$$\nabla_{\vec{B}} \hat{H} = \mu \nabla_{\vec{B}} (\vec{B}\vec{J}) = \mu \vec{J}$$

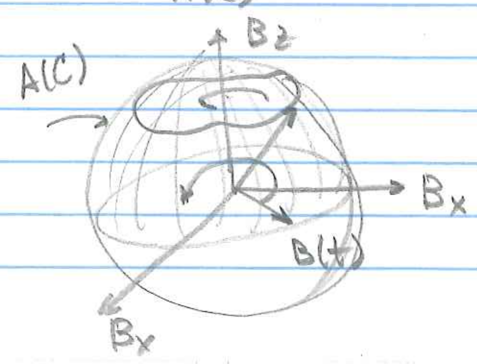
We need to calculate

$$\mu^2 \sum_{m' \neq m} \frac{\overbrace{\langle m|\vec{J}|m'\rangle \times \langle m'|\vec{J}|m\rangle}^{\sim \hbar^2}}{\underbrace{(E_m - E_{m'})^2}_{(\hbar \mu B_0)^2}} = \frac{i m \vec{e}_z}{B_0^2} = \frac{i m}{|B_0|^2} \vec{e}_{\vec{B}}$$

since $\vec{J} = \hat{J}_+ \vec{e}_+ + \hat{J}_- \vec{e}_- + J_z \vec{e}_z$ $\quad m' = \pm m$, and each $\langle m|J|m'\rangle$ vector is in x-y plane, so that the vector product is in z-direction

Berry phase $\qquad$ singularity at $B_0 = 0$

$$\gamma = -\int_{A(C)} \frac{m \vec{B}}{|B|^3}\, d\vec{a}_{\vec{B}}$$



Rotating magnetic field
C – circle of radius B_0
$d\vec{a}_{\vec{B}} = B_0^2\, \vec{B}/B_0\, d\Omega$

$\gamma = -m \cdot \Omega_C$
solid angle

Phase depends on the value of the original angular momentum state

$J_z \; j = 1/2 \qquad \gamma_{\pm} = \pm \frac{1}{2} \Omega$

For an experiment with phase sensitivity (interferometry!) the Berry phase can be measured