Adiabatic evolution of $\hat{H}$ and accumulation of Geometric phase.

$$\hat{H} \equiv \hat{H}(t) \Rightarrow \qquad \hat{H}(t)\,|n\,t\rangle = E_{nt}\,|n\,t\rangle \longrightarrow (1) \quad \{E_{nt}, |n\,t\rangle\} \rightarrow \text{instantaneous eigenvalues and eigenstate.}$$

To study the time evolution of an arbitrary state $|\alpha\,t\rangle$ under the influence of $\hat{H}(t)$ we need to solve:

$$i\hbar \frac{\partial}{\partial t}|\alpha t\rangle = \hat{H}(t)\,|\alpha t\rangle. \longrightarrow (2)$$

we can expand $|\alpha t\rangle = \sum_m c_m(t)\,|m t\rangle.$

$$(2) \Rightarrow \quad i\hbar \sum_m \left[\dot{c}_m(t)\,|m t\rangle + c_m(t)\,\frac{\partial |m t\rangle}{\partial t}\right] = \sum_n c_m(t)\,E_{mt}\,|m t\rangle.$$

$\langle j t|$ on both sides:

$$i\hbar\,\dot{c}_j(t) + \sum_m c_m(t)\,\langle j t|\frac{\partial |m t\rangle}{\partial t} = -i\,c_j(t)\,E_{jt}/\hbar$$

$$\Rightarrow \quad \dot{c}_j(t) = c_j\left[-i\frac{E_j}{\hbar} + \langle j t|\frac{\partial}{\partial t}|j t\rangle\right] - \sum_{m\neq j} c_m(t)\,\langle j t|\frac{\partial}{\partial t}|m t\rangle. \longrightarrow (3)$$

① → Recall $H(t)|nt\rangle = E_{nt}|nt\rangle$

$\frac{\partial}{\partial t}$ on both sides $\Rightarrow$ $\dot{H}(t)|nt\rangle + H(t)\frac{\partial|nt\rangle}{\partial t} = E_{nt}\frac{\partial|nt\rangle}{\partial t}$

$\langle jt|$ both sides $\Rightarrow$ $\langle jt|\dot{H}(t)|nt\rangle + \underbrace{\langle jt|H(t)}_{E_{jt}}\frac{\partial}{\partial t}|nt\rangle = E_{nt}\langle jt|\frac{\partial}{\partial t}|nt\rangle$

$\Rightarrow$ $\langle jt|\dot{H}(t)|nt\rangle = (E_{nt} - E_{jt})\langle jt|\frac{\partial|nt\rangle}{\partial t}$

$\Rightarrow$ $\langle jt|\frac{\partial}{\partial t}|mt\rangle = \dfrac{\langle jt|\dot{H}(t)|nt\rangle}{E_{nt} - E_{jt}}$

③ → $\dot{c}_j(t) = c_j\left(\frac{-iE_j}{\hbar}\right) - c_j\langle jt|\frac{\partial}{\partial t}|jt\rangle - \sum_{m\neq j} c_m(t)\,\dfrac{\langle jt|\dot{H}(t)|nt\rangle}{E_{nt} - E_{jt}}$

Adiabatic approximation :

$$\frac{\langle jt|\dot{H}(t)|nt\rangle}{E_{nt} - E_{jt}} \ll \langle jt|\frac{\partial}{\partial t}|jt\rangle \approx \frac{E_{jt}}{\hbar}$$

$\Rightarrow$ $\underbrace{\langle jt|\dot{H}(t)|nt\rangle\left(\frac{\hbar}{E_{jt}}\right)}$ $\ll E_{nt} - E_{jt}$

$\Rightarrow$ Change of $\hat{H}$, ie $\langle jt|\hat{H}|nt\rangle$ over the natural time scale of states $\ll$ Energy separation

$\Rightarrow$ Negligible mixing of states.

$$\Rightarrow \dot{c}_j(t) = \frac{-iE_{jt}c_j}{\hbar} - c_j \langle jt|\frac{\partial}{\partial t}|jt\rangle$$

$$\Rightarrow \frac{d \ln c_j(t)}{dt} = -\frac{iE_{jt}}{\hbar} - \langle jt|\frac{\partial}{\partial t}|jt\rangle$$

$$\Rightarrow \ln c_j(t) = \left(\frac{-i}{\hbar}\int_0^t E_{jt'}\, dt'\right) - \int_0^t \langle jt'|\frac{\partial}{\partial t'}|jt'\rangle\, dt'$$

$$\Rightarrow c_j(t) = e^{i\theta_j(t)}\, e^{i\gamma_j(t)} \quad ; \quad \theta_j(t) = -\frac{1}{\hbar}\int_0^t E_j(t')\, dt'$$

$$\gamma_j(t) = i\int_0^t \langle jt'|\frac{\partial}{\partial t'}|jt'\rangle\, dt'$$

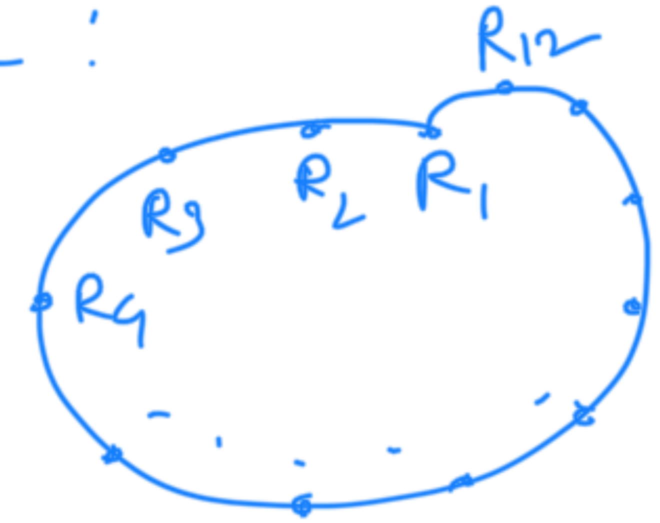
Now $\langle jt|jt\rangle = 1$

$$\Rightarrow \left(\langle jt|\frac{\partial}{\partial t}|jt\rangle\right) + \left(\langle jt|\frac{\partial}{\partial t}|jt\rangle\right)^* = 0$$

$$\Rightarrow \underbrace{\langle jt|\frac{\partial}{\partial t}|jt\rangle}_{\text{purely imaginary}}$$

$\therefore \gamma_j(t) \longrightarrow$ REAL

Parameter space :



Let $H = H_0 + V(\vec{r}, \{R(t)\})$; $\{R(t)\} \to \{R_1(t), R_2(t), R_3(t), \dots\}$ → Defines a parameter space

Parameter can independently vary.

$$\therefore\ d|n R\rangle = \sum_i \frac{\partial |n\{R\}\rangle}{\partial R_i}\, dR_i$$

$$\frac{d|nR\rangle}{dt} = \sum_i \frac{\partial |n\{R\}\rangle}{\partial R_i}\frac{dR_i}{dt} = \nabla_R |n\{R\}\rangle \cdot \frac{d\vec{R}}{dt}$$; $\vec{R}$: vector of parameters.

$\therefore$ Let $\{R_i\} \longrightarrow \{R_f\}$

$$\therefore\ \gamma_n = i\int_{\{R_i\}}^{\{R_f\}} \langle n\{R\}| \left(\nabla_R |n\{R\}\rangle \cdot \frac{d\vec{R}}{dt}\right) dt = i\int_{\{R_i\}}^{\{R_f\}} \langle n\{R\}|\nabla_R|n\{R\}\rangle \cdot d\vec{R}$$

line element in $\{R\}$ space

Note: $|n\{R\}\rangle \equiv |n\vec{R}\rangle$, $\vec{R}$ → vector of parameter

Now if H returns to itself after evolving in a closed path in the parameter space spanned by $\{R\}$ then

$$\gamma_n(C) = i \oint \langle n\vec{R} | \nabla_R | n\vec{R} \rangle \cdot d\vec{R} \longrightarrow \text{Berry's phase}$$

closed loop

(Gauge invariant) we will show below.

$$= i \iint \left(\nabla_R \times \langle n\vec{R} | \nabla_R | n\vec{R} \rangle \right) \cdot \vec{ds}$$

$\therefore \gamma_n(C) \to$ flux enclosed by a closed loop

and $\nabla_R \times \langle n\vec{R} | \nabla_R | n\vec{R} \rangle$ is effectively a magnetic field

Gauge Invariance

If we arbitrarily add a phase varying with $\vec{R}$ with $|n\vec{R}\rangle$ $\longrightarrow$ Gauge freedom

$$|n\vec{R}\rangle \longrightarrow |\widetilde{n\vec{R}}\rangle = e^{i\delta(\vec{R})} |n\vec{R}\rangle$$

then $\widetilde{A}_n(\vec{R}) = i \langle \widetilde{n\vec{R}} | \nabla_R | \widetilde{n\vec{R}} \rangle = i \langle n\vec{R} | e^{-i\delta(\vec{R})} \left(i\nabla\delta(\vec{R})\, e^{i\delta(\vec{R})} |n\vec{R}\rangle + e^{i\delta(\vec{R})} \nabla_R |n\vec{R}\rangle \right)$

$$= -\nabla\delta(\vec{R}) + A_n(\vec{R})$$

$$\therefore \widetilde{\gamma}_n(C) = \iint \nabla_R \times \widetilde{A}_n(\vec{R}) \cdot \vec{ds}$$

$$= \iint \nabla_R \times \left(A_n(\vec{R}) - \nabla\delta(\vec{R}) \right) \cdot \vec{ds}$$

$$= \iint \nabla_R \times A_n(\vec{R}) \cdot \vec{ds} = \gamma_n(C) \longrightarrow \text{Gauge invariance.}$$

∴ The effective interpretation of Berry phase is that of "some kind" of gauge invariant flux due to an "effective" magnetic field due to evolution of the Hamiltonian in a closed path in parameter space.

Effective vector potential:

$$\xi_n(t) \longrightarrow \vec{A}_n(\vec{R}) = i\langle n\vec{R}|\nabla_R|n\vec{R}\rangle \rightarrow \underline{\text{Berry Connection}}$$

Effective magnetic field:

$$\nabla_{\vec{R}} \times \vec{A}_n(R) = \nabla_{\vec{R}} \times \langle n\vec{R}|\nabla_{\vec{R}}|n\vec{R}\rangle$$
$$= \left(\nabla_{\vec{R}}\langle n\vec{R}|\right) \times \left(\nabla_R|n\vec{R}\rangle\right) \rightarrow \underline{\text{Berry curvature}}$$

Gauge invariant flux:

$$\gamma_n(c) = i\oint \langle n\vec{R}|\nabla_{\vec{R}}|n\vec{R}\rangle \cdot \vec{dR} \longrightarrow \underline{\text{Berry phase}}$$

<u>Practical calculation:</u>

$$|n\vec{R}+\vec{\Delta R}\rangle = |n\vec{R}\rangle + \nabla_{\vec{R}}|n\vec{R}\rangle \cdot \vec{\Delta R}$$

$$\langle n\vec{R}|n\vec{R}+\vec{\Delta R}\rangle \simeq 1 + \langle n\vec{R}|\nabla_{\vec{R}}|n\vec{R}\rangle \cdot \vec{\Delta R}$$

$$= 1 - i^2 \langle n\vec{R}|\nabla_{\vec{R}}|n\vec{R}\rangle \cdot \vec{\Delta R}$$

$$= e^{-i\left(i\langle n\vec{R}|\nabla_{\vec{R}}|n\vec{R}\rangle \cdot \vec{\Delta R}\right)}$$

$$i\ln\langle n\vec{R}|n\vec{R}+\vec{\Delta R}\rangle = i\langle n\vec{R}|\nabla_{\vec{R}}|n\vec{R}\rangle \cdot \vec{\Delta R}$$

$$\therefore\ i\sum_{\substack{R_i \\ \vec{R}_f+\vec{\Delta R}=\vec{R}_i}}^{R_f} \ln\langle n\vec{R}|n\vec{R}+\vec{\Delta R}\rangle = i\sum_{\substack{R_i \\ \vec{R}_f+\vec{\Delta R}=\vec{R}_i}}^{R_f}\langle n\vec{R}|\nabla_R|n\vec{R}\rangle \cdot \vec{\Delta R}$$

$$\Rightarrow \gamma(c) = i\oint \langle n\vec{R}|\nabla_R|n\vec{R}\rangle \cdot d\vec{R} \simeq i\ln\prod_{R_i}^{R_f}\langle n\vec{R}|n\vec{R}+\vec{\Delta R}\rangle$$