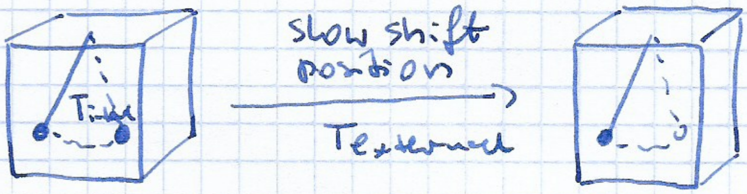
IV BERRY PHASE AND TOPOLOGICAL STATES IN QUANTUM MECHANICS

§ 1. Adiabatic approximation

after D.J. Griffiths
Quantum mechanics

•) Adiabatic processes

classical pendulum



adiabatic process if $\boxed{T_{internal} \ll T_{external}}$

Example $\quad T = 2\pi\sqrt{\frac{L}{g}}$ and change slowly $L = L(t)$

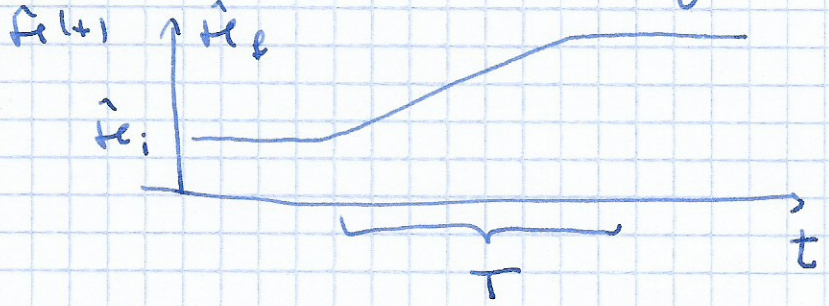
if $\frac{1}{L(t)} \frac{dL(t)}{dt} \ll \frac{1}{T} \longrightarrow \boxed{T(t) = 2\pi\sqrt{\frac{L(t)}{g}}}$

Example $\quad$ Born-Oppenheimer approximation

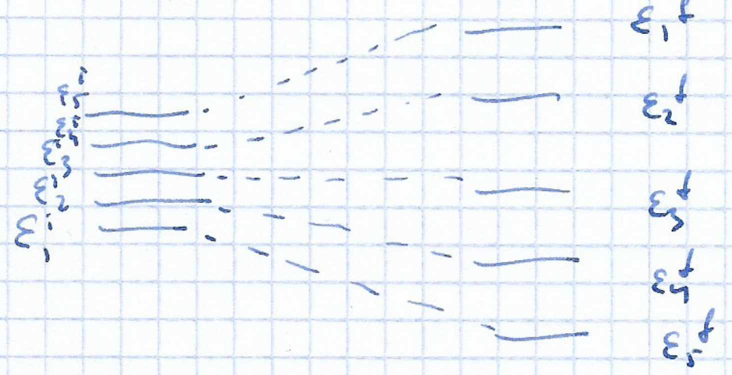
$$\psi(\bar{r}_e, \bar{R}_i) = \psi_{el}(\bar{r}_e) \cdot \psi_i(\bar{R}_i)$$

• Adiabatic theorem in quantum mechanics

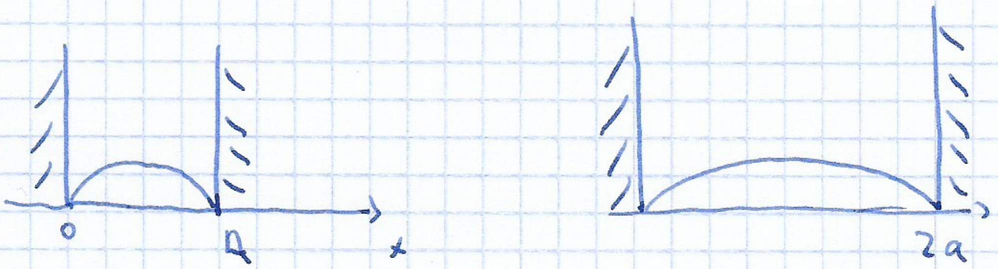
$\hat{H}$ is changed gradually from $\hat{H}_i$ to $\hat{H}_f$



Theorem: If a system was in nth eigenstate of $\hat{H}_i$ then it remains in nth eigenstate of $\hat{H}_f$ [Ehrenfest, Born, Fock - 1928]



Example

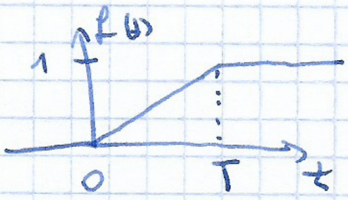


$$\psi_i(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi}{a}x\right) \xrightarrow[\text{slow}]{} \psi_f(x) = e^{i\varphi}\sqrt{\frac{1}{a}}\,\sin\left(\frac{\pi}{2a}x\right)$$

proof

$$\hat{H}(t) = \hat{V} f(t)$$

"small"



states are not degenerate

$$\Psi_n(0) = \psi_n^i \longrightarrow \Psi(t)$$

eigenstate of $\hat{H}_i$

If $f(t)$ changes slowly

$$|\langle \Psi(T) | \psi_m^f \rangle|^2 = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}$$

eigenstate of $\hat{H}_f$

→ 1st order of perturbation without time

$$\boxed{\psi_m^f = \psi_m + \sum_{k \neq m} \frac{V_{km}}{E_m - E_k} \psi_k} \quad (*)$$

$V_{km} = \langle \psi_k | \hat{V} | \psi_m \rangle$

states and energies at $t = 0$

→ 1st order of perturbation with time

$$\boxed{\Psi(t) = \sum_l c_l(t)\, \psi_l\, e^{-i \frac{E_l t}{\hbar}}}$$

$$c_l = \begin{cases} 1 - \frac{i}{\hbar} V_{nn} \int_0^t f(t')\, dt' & l = n \\ -\frac{i}{\hbar} V_{ln} \int_0^t f(t') e^{i(E_l - E_n)t'/\hbar}\, dt' & l \neq n \end{cases}$$

Note: $e^{i \frac{E_l - E_n}{\hbar} t} = -\frac{i\hbar}{E_l - E_n} \frac{d}{dt} e^{i \frac{E_l - E_n}{\hbar} t}$

and integrates by parts $(l \neq n)$

$$c_l(t) = -\frac{V_{ln}}{E_l - E_n} \int_0^t f(t') \frac{d}{dt'} \left[e^{i \frac{E_l - E_n}{\hbar} t'} \right] dt' =$$

$$= -\frac{V_{ln}}{E_l - E_n} \left[f(t) e^{i \frac{E_l - E_n}{\hbar} t'} \Big|_0^t - \int_0^t \frac{df}{dt'} e^{i \frac{E_l - E_n}{\hbar} t'} dt' \right]$$

$f(0) = 0$

adiabatic condition $T_{ext} \gg T_{int}$

$$\boxed{\frac{1}{T_{ext}} = \frac{1}{f} \frac{df}{dt} \ll \frac{|E_l - E_n|}{\hbar} = \frac{1}{T_{int}}}$$

adiabatic approximation valid if

$$\boxed{\frac{\partial f}{dt} \ll \frac{|E_l - E_n|}{\hbar} f}$$

$$e^{i\frac{E_l}{\hbar}T} \cdot e^{-i\frac{E_l T}{\hbar}} = 1$$

$$(*) \quad \boxed{\Psi(T) = \left[\left(1 - i \frac{V_{nn} A}{\hbar}\right) \psi_n - \sum_{l \neq n} \frac{V_{ln}}{E_l - E_n} \psi_l \right] e^{-i\frac{E_n T}{\hbar}}}$$

$A = \int_0^T f(t)\, dt$ - area of $f(t)$ from 0 to T

$f(T) = 1$

compute the scalar product $*)$ & $(**)$

$$\langle \Psi(T) | \psi_m^f \rangle = \left[\left(1 + i \frac{V_{nn}^* A}{\hbar}\right) \langle \psi_n | - \sum_{l \neq n} \frac{V_{ln}^*}{E_l - E_n} \langle \psi_l | \right] e^{\frac{i E_n T}{\hbar}} \cdot$$

$$\overbrace{O(V_{nm})} \left[|\psi_m\rangle + \sum_{k \neq m} \frac{V_{km}}{E_m - E_k} |\psi_k\rangle \right] =$$

$$= \left[\left(1 + i \frac{V_{nn}^* A}{\hbar}\right) \underbrace{\langle \psi_n | \psi_m \rangle}_{\delta_{nm}} - \sum_{l \neq n} \underbrace{\frac{V_{lm}^*}{E_l - E_n}}_{O(V_{nm})} \underbrace{\langle \psi_l | \psi_m \rangle}_{\delta_{lm}} \right] e^{\frac{i E_n T}{\hbar}} + O(V_{nm}^2)$$

up to $O(1)$ terms

$$\boxed{\langle \Psi(T) | \psi_m^f \rangle = \begin{cases} \left(1 + i \frac{V_{nn} A}{\hbar}\right) e^{\frac{i E_n T}{\hbar}} & n = m \\ 0 & n \neq m \end{cases}}$$

If $\hat{V}$ not "small" we can split $T \to \frac{T}{N}$ such that $\left(\frac{\hat{V}}{N}\right)$ - "small"

$\square$

J.M.
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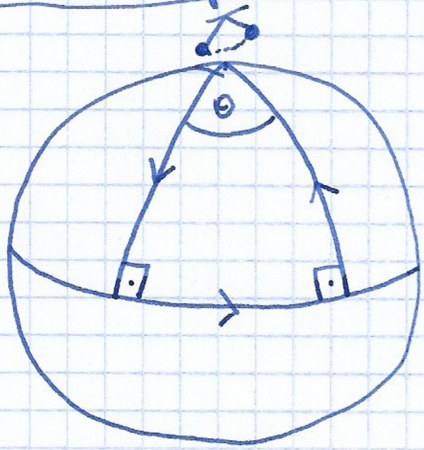
§ 2. Berry (geometric) phases

Anholonomy – a failure to come back to the exact same initial state after performing parallel transport / process along a closed path in a curved space

Classical example



parallel / adiabatic transport of a pendulum
meridian – equator – meridian

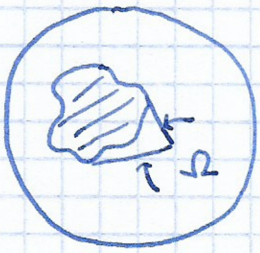
It swings in a new plane making θ angle with the old one

θ is the solid angle.

Indeed, the area A

$$A = \underbrace{\tfrac{1}{2}}_{\text{north hemisphere}} \underbrace{\left(\frac{\theta}{2\pi}\right)}_{\text{fraction of the hemisphere}} 4\pi R^2 = \theta R^2 \rightarrow \boxed{\Omega = \frac{A}{R^2} = \theta}$$

In general



$\theta = \Omega$ will not depend on a particular shape

→ Foucault pendulum
Hannay's angle ↔ geometric phase

geometric phase in quantum mechanics

Let ~~[illegible]~~ $\hat{H}\,\psi_n(x) = E_n\,\psi_n(x)$

$\hat{H}$ time independent

$$\underbrace{\Psi_n(x,t) = \psi_n(x)\,e^{-i\frac{E_n t}{\hbar}}}_{\text{oscillation}} \leftarrow \text{stationary solution}$$

Let $\hat{H} = \hat{H}(t)$ changes in time

then $\hat{H}(t)\,\psi_n(x,t) = E_n(t)\,\psi_n(x,t)$

time dependent

Theorem

If $\hat{H}(t)$ changes slowly (adiabatically) then the n-th quantum state remains the n-th quantum state up to a phase

$$\boxed{\Psi_n(x,t) = \psi_n(x,t)\,e^{-\frac{i}{\hbar}\int^t E_n(t')\,dt'}\,e^{i\gamma_n(t)}}$$

depends on time due to parameters in $\hat{H}(t)$

geometric phase

only in adiabatic limit

$$\boxed{\theta_n(t) = -\frac{1}{\hbar}\int^t E_n(t')\,dt'} \leftarrow \text{dynamical phase}$$

[generalization of $-\frac{E_n t}{\hbar}$]

$\Psi_n(x,t)$ obeys Schrödinger eq.

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi_n(x,t) = \hat{H}(t)\,\Psi_n(x,t)}$$

if γ_n fulfills some conditions

Df. any additional phase $\gamma_n(t)$, allowed by an adiabatic theorem, is called a geometric phase

This phase was regarded as unimportant until M. Berry realized that in a cyclic processes
$\hat{H}(t+T) = \hat{H}(t)$
the difference of $\gamma_n(t)$ and $\gamma_n(t+T)$ is observable!

check out $\quad i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \hat{H}(t)\Psi(x,t)$

$$\Psi_n(x,t) = \psi_n(x,t)\, e^{i\theta_n(t)} e^{i\gamma_n(t)}$$

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

$$= \hat{H}\psi_n e^{i\theta_n} e^{i\gamma_n} = \underline{E_n \psi_n e^{i\theta_n} e^{i\gamma_n}}$$

because $\quad \frac{d}{dx}\int^x f(y)\,dy = f(x)$

$$\frac{d}{dt} e^{-\frac{i}{\hbar}\int^t E_n(t')dt'} = -\frac{i}{\hbar}\frac{d}{dt}\int^t E(t')dt'\, e^{i\theta_n} = -\frac{i}{\hbar} E_n(t) e^{i\theta_n}$$

$\Rightarrow$ the condition on $\gamma_n(t)$

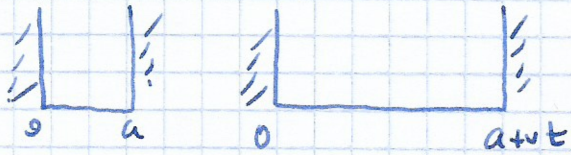
(*) $\quad \frac{\partial \psi_n}{\partial t} + i\frac{d\gamma_n}{dt}\psi_n = 0 \quad \Big| \int \psi_n^*(x)\,dx$

if $\psi_n(x)$ is normalized

$$\Rightarrow \quad \boxed{\frac{d\gamma_n}{dt} = i\left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial t}\right\rangle}$$

Note, that without $\gamma_n(t)$ the ansatz $\psi_n e^{i\theta_n}$ would not work at all.

Typically, $\psi_n(x,t)$ depends on t via some parameter $R(t)$. [E.g. width of a quantum well $w(t) = a + vt$]



Then

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R} \frac{dR}{dt}$$

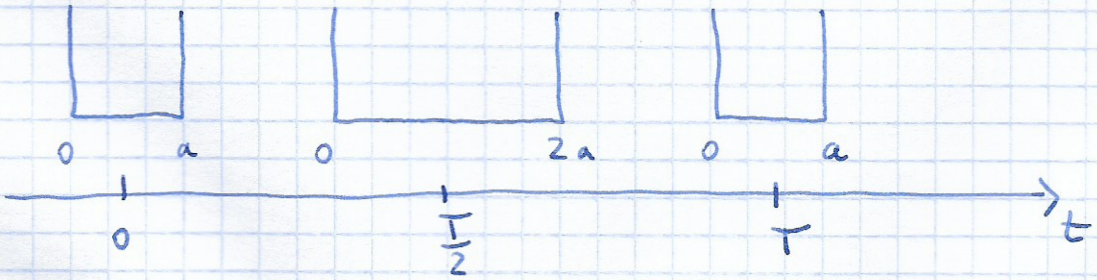
$$\Rightarrow \quad \frac{d\gamma_n}{dt} = i \left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial R} \right\rangle \frac{dR}{dt} \quad / \int dt$$

$$\boxed{\gamma_n(t) = i \int_0^t \left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial R} \right\rangle \frac{dR}{dt'} dt' = i \int_{R_i}^{R_f} \left\langle \psi_n \middle| \frac{\partial \psi_n}{\partial R} \right\rangle dR}$$

If $R_i = R(0)$ and $R_f = R(T)$ and

$$\hat{H}(0) = \hat{H}(T) \rightarrow R_f = R_i \rightarrow \underline{\gamma_n(T) = 0}$$

Example



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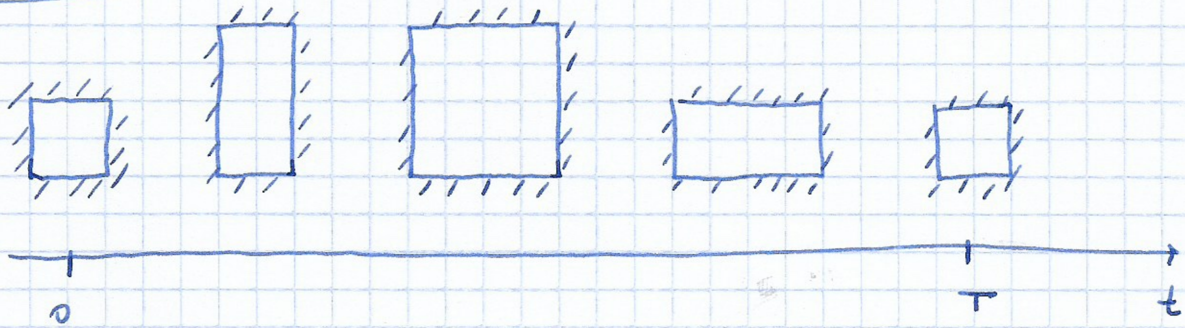
More interesting is the problem where the parameter space is multidimensional

$$\bar{R}(t) = \underbrace{\left(R_1(t),\ R_2(t),\ \dots,\ R_N(t)\right)}_{N\text{ - dimensions}}$$

Example



$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R_1}\frac{dR_1}{dt} + \frac{\partial \psi_n}{\partial R_2}\frac{dR_2}{dt} + \dots + \frac{\partial \psi_n}{\partial R_N}\frac{dR_N}{dt} = \left(\bar{\nabla}_R \psi_n\right)\cdot \frac{d\bar{R}}{dt}$$

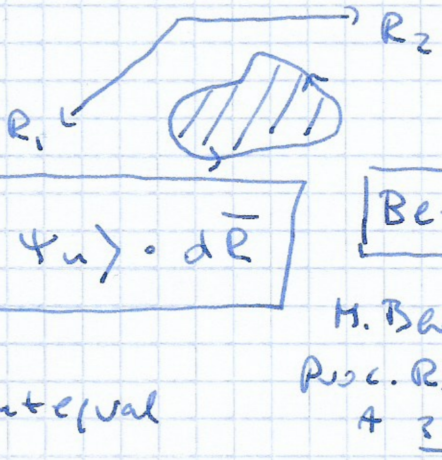
N - dimensional gradient

$\bar{\nabla} = (\partial_{R_1}, \partial_{R_2} \dots \partial_{R_N})$

$$\boxed{\gamma_n(t) = i \int_{\bar{R}_i}^{\bar{R}_f} \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n \rangle \cdot d\bar{R}}$$

Geometric - phase

If $\hat{H}(0) = \hat{H}(T)$



$$\boxed{\gamma_n(T) = i \oint \langle \psi_n | \bar{\nabla}_{\bar{R}} \psi_n \rangle \cdot d\bar{R}}$$

Berry phase

M. Berry
Proc. R. Soc. London A 392, 45 (1984)

typically this contour integral is non-zero

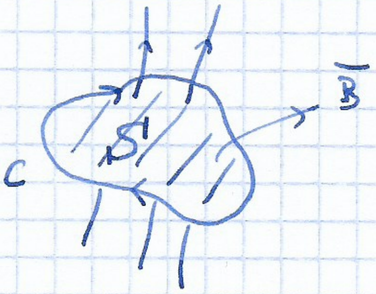
$\gamma_n(T)$ – depends on a path (shape) but not on how fast the system evolved, therefore Berry phase does not depend on T!

(geometric, topological)

In contrast, $\theta_n(T) = \int^T E_n(t)\,dt$ – depends on T.

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?

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

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

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

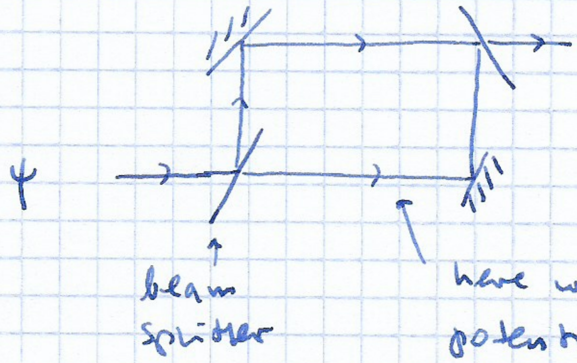
$\langle \Psi_n | \bar{\nabla}_{\bar{R}} \Psi_n \rangle$ – pure imaginary

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

□

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

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

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

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

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

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

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

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

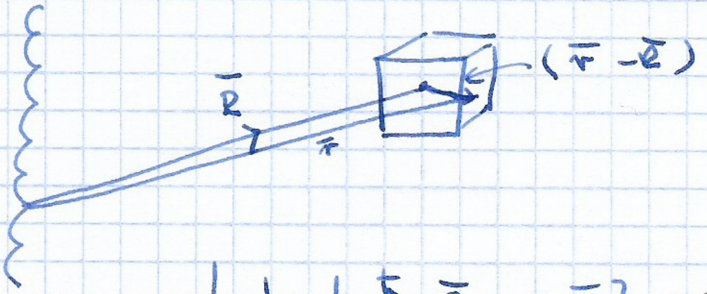
Note, formally eq. (*) on p. 76 should read

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

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 $V(\bar r - \bar R)$



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

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

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

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

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

$\downarrow$

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

$\bar\nabla_{\bar R} = -\bar\nabla_{\bar r}$; $\bar\nabla_{\bar r} = \frac{i}{\hbar}\hat{\bar p}$

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

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