Agenda for Today

Combine Berry phase + B. Curvature with solid state physics

→ As one applies a magnetic/electric field, one tunes the wavevector $\vec{k}$ & this corresponds exactly to the type adiabatic evolution with vector $\vec{k}$ in place of parameter λ.

→ phrasing: we want solutions of periodic in k-space part of wave function $u^{n}_{k,\sigma}(\vec{r})$ of the Bloch wavefunction $\psi^{n}_{k,\sigma}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u^{n}_{\vec{k},\sigma}(\vec{r})$

• The $\vec{k}$ dependent effective hamiltonian for such matters is $\underline{\underline{H_{\vec{k}} = e^{-i\vec{k}\cdot\vec{r}}\, H\, e^{ikr}}}$ → this is then a function of parameter $\vec{k}$!

s.t. $u_{n,k}(\vec{r})$ obeys

$$\left[\frac{\hbar^2}{2m}\left(\underbrace{\vec{k}}_{\text{parameter of the hamiltonian}}-i\nabla\right)^2 + V(\vec{r})\right] u^{n}_{k,\sigma}(\vec{r}) = \mathcal{E}^{n}_{k,\sigma}\, u^{n}_{k,\sigma}(\vec{r})$$

→ now when an electron follows a trajectory in k-space, ∃ a corresponding Berry connection

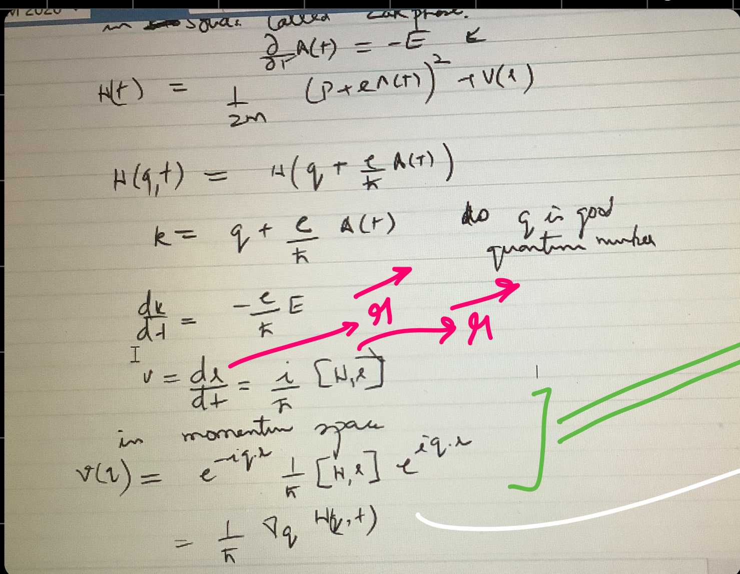
$$\vec{A}^{n}_{\sigma}(\vec{k}) = i\langle u^{n}_{k,\sigma} | \nabla_k | u^{n}_{k,\sigma}\rangle$$

s.t.

$$\left[u_{\vec{k}}(\vec{r})\right]_{\vec{k}+\delta\vec{k}} = e^{i\vec{A}(\vec{k})\cdot\delta\vec{k}}\, u_{k+\delta k}(\vec{r})$$

& subsequently we can have a non-zero B. curv &
B. phase.

Case study :- e^-'s in a band.



called ... phase.

$$\frac{\partial}{\partial t} A(t) = -E$$

$$H(t) = \frac{1}{2m}\left(p + eA(t)\right)^2 + V(r)$$

$$H(q,t) = H\left(q + \frac{e}{\hbar} A(t)\right)$$

$$k = q + \frac{e}{\hbar} A(t)$$ so q is good quantum number

$$\frac{dk}{dt} = -\frac{e}{\hbar} E$$

$$v = \frac{dr}{dt} = \frac{i}{\hbar}[H, r]$$

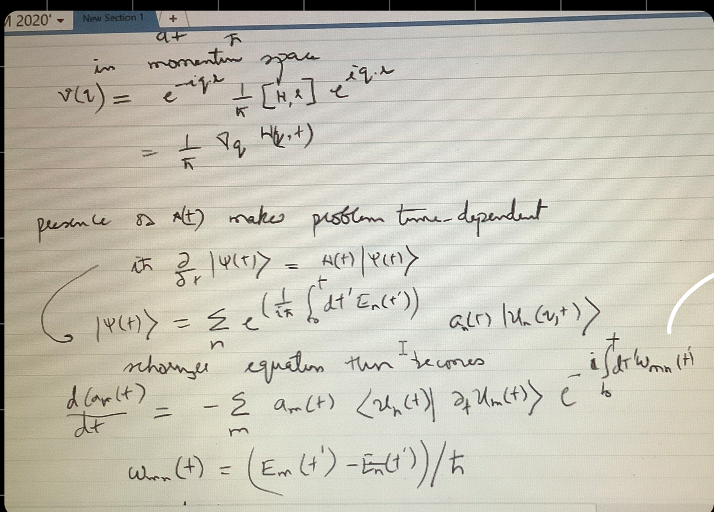
in momentum space

$$v(q) = e^{-iq\cdot r} \frac{1}{\hbar}[H, r]\, e^{iq\cdot r}$$

$$= \frac{1}{\hbar} \nabla_q H(q,t)$$

Momentum space rep.

following Shin-shen's book



in momentum space

$$v(q) = e^{-iq\cdot r} \frac{1}{\hbar}[H, r]\, e^{iq\cdot r}$$

$$= \frac{1}{\hbar} \nabla_q H(q,t)$$

presence of $A(t)$ makes problem time-dependent

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

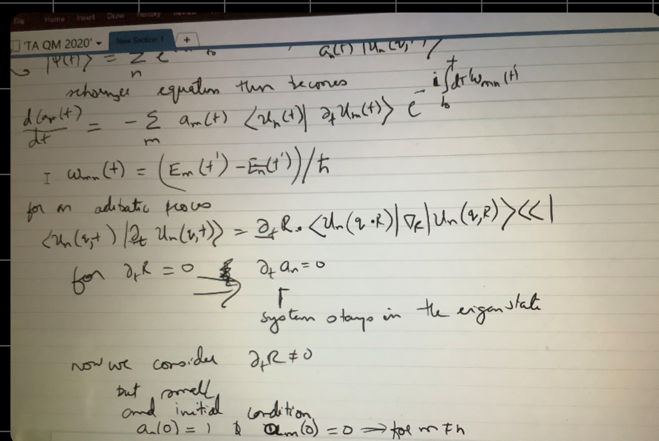
$$|\psi(t)\rangle = \sum_n e^{\left(\frac{1}{i\hbar}\int_{t_0}^{t} dt' E_n(t')\right)} a_n(t) |u_n(q,t)\rangle$$

schrodinger equation then becomes

$$\frac{d(a_n(t))}{dt} = -\sum_m a_m(t) \langle u_n(t)| \partial_t u_m(t)\rangle\, e^{-i\int_{t_0}^{t} dt' \omega_{mn}(t')}$$

$$\omega_{mn}(t) = \left(E_m(t') - E_n(t')\right)/\hbar$$

$E_{n,m}$



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for an adiabatic process

$$\langle u_n(q,t) | \partial_t u_n(q,t)\rangle = \partial_t R \cdot \langle u_n(q,R)| \nabla_R | u_n(q,R)\rangle \ll 1$$

for $\partial_t R = 0 \implies \partial_t a_n = 0$

system stays in the eigenstate

now we consider $\partial_t R \neq 0$

but small

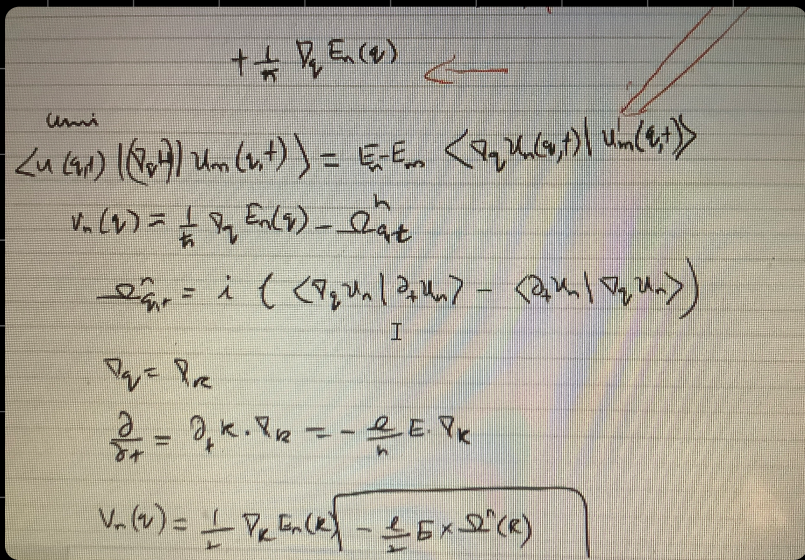
and initial condition

$a_n(0) = 1$ & $a_m(0) = 0 \implies$ for $m \neq n$

So essentially shen's book.

$|u_n(t)\rangle \to |u_n(q,t)\rangle$ — correction

• $v_n(q) = \frac{\nabla_q E_n(q)}{\hbar} - \Omega^n_{q,t}$


$+\frac{1}{\hbar}\nabla_q E_n(q)$

u_m

$\langle u(q,t)|(\nabla_q H)|u_m(q,t)\rangle = (E_n - E_m)\langle \nabla_q u_n(q,t)|u_m(q,t)\rangle$

$v_n(q) = \frac{1}{\hbar}\nabla_q E_n(q) - \Omega^n_{q t}$

$\Omega^n_{q,t} = i\left(\langle\nabla_q u_n|\partial_t u_n\rangle - \langle\partial_t u_n|\nabla_q u_n\rangle\right)$

$\nabla_q = \nabla_k$

$\frac{\partial}{\partial t} = \partial_t k\cdot\nabla_k = -\frac{e}{\hbar}E\cdot\nabla_k$

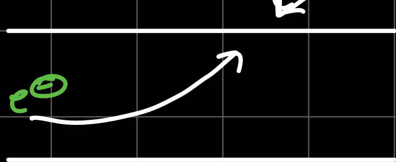
$v_n(q) = \frac{1}{\hbar}\nabla_k E_n(k) \boxed{- \frac{e}{\hbar}E\times\Omega^n(k)}$

∴ new term

$v_n(\vec{q}) = \frac{1}{\hbar}\nabla_k E_n(\vec{k}) - \frac{e}{\hbar}\vec{E}\times\Omega^n(\vec{k})$

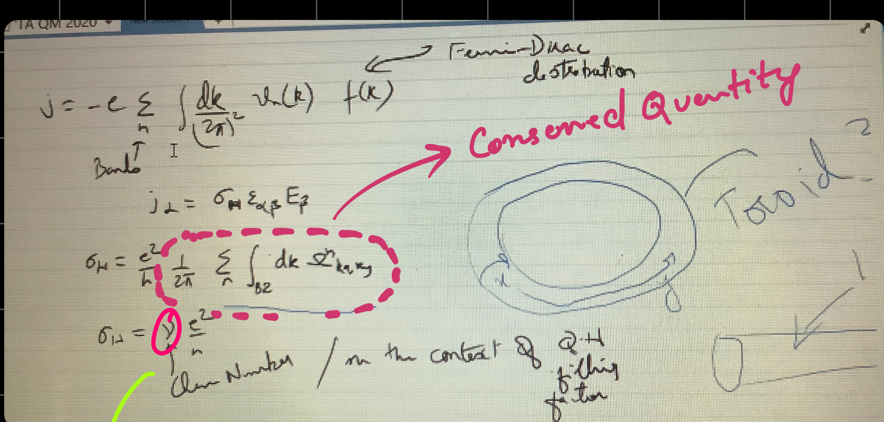
⇓

it'll try to drift the electron to one side over the other.



Tangible consequence :- If you have a non-zero Berry phase, then it'll have a drift response on the electron.

this depends intimately on the Quantum nature of the problem.


TA QM 2020

$j = -e\sum_n \int \frac{dk}{(2\pi)^2} v_n(k)\, f(k)$ ← Fermi-Dirac distribution

Bands

$j_\perp = \sigma_H \epsilon_{\alpha\beta} E_\beta$

Conserved Quantity

$\sigma_H = \frac{e^2}{h}\frac{1}{2\pi}\sum_n\int_{BZ} dk\, \Omega^n_{k_x k_y}$

$\sigma_H = \nu \frac{e^2}{h}$

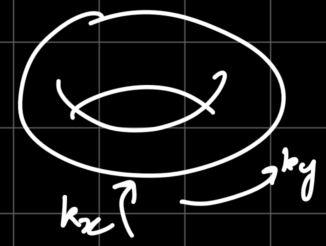
Chern Number / in the context of QH filling factor

Toroid?

not derived.

for integer QHall, chern number is same as filling factor.

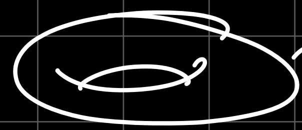
#



$\sigma = \nu \frac{e^2}{\hbar}$

Chern # is an invariant over a <u>surface</u>.

Related to Gauss bonnet theorem.



unless & until there's a tear in the system!

<u>Wouldn't disorder trouble this?</u>

↳ @ Atland.

$\boxed{\text{Disorder vs Topology}}$ → see flow diagram of TIns

But what gives? We didn't take the Berry curvature <u>earlier</u>.

Turns out Berry Curvature is 0 for most materials.

So under what conditions is Berry curvature non-zero?

<u>Symmetry</u> <u>props</u> of <u>Hamiltonian</u>

Time reversal symmetry

Inversion symmetry.

$k \to -k$

① $\underbrace{\Omega(k) = -\Omega(-\vec{k})}_{\text{of Berry curvature}}$

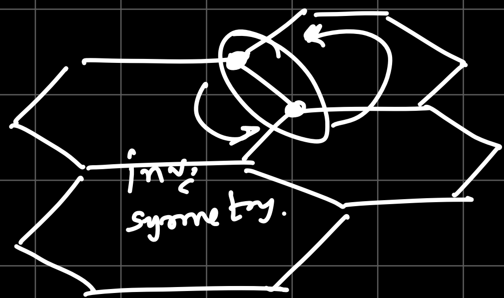
② $\Omega(\vec{k}) = \Omega(-\vec{k})$

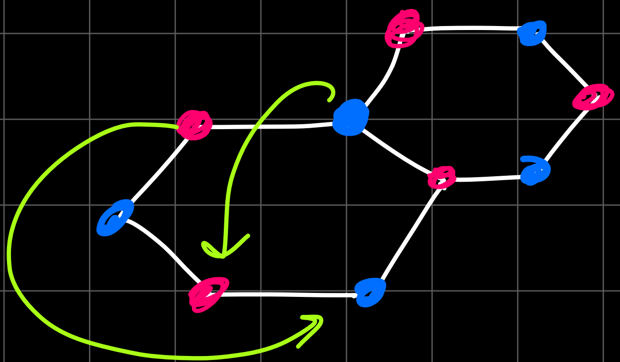
if both hold, then B.C. <u>vanish</u>.

If system has TRS, then Chern # = 0

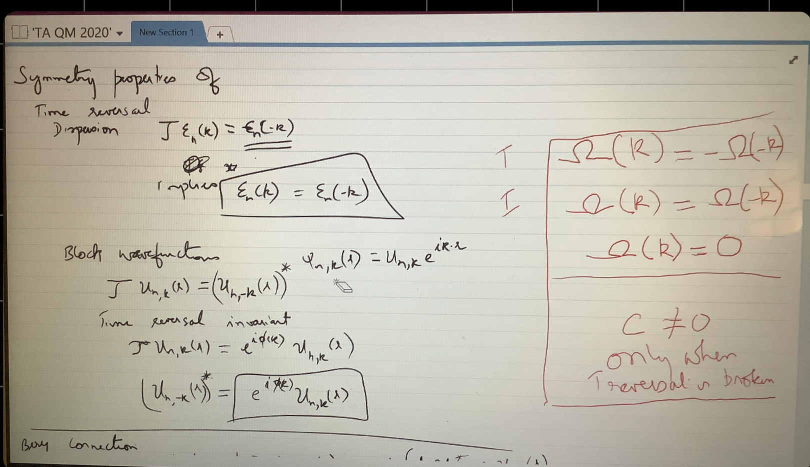
TRS → break by introducing magnetism.

I symmetry ⇒ strain / defects / Lattice symmetry





→ under inv. breaking then we automatically generate **Berry phase**.


'TA QM 2020'
New Section 1

Symmetry properties of
Time reversal
Dispersion $T\,\varepsilon_n(k) = \varepsilon_n(-k)$

implies $\boxed{\varepsilon_n(k) = \varepsilon_n(-k)}$

Block wavefunctions $\psi_{n,k}(r) = u_{n,k}\, e^{ik\cdot r}$

$T\, u_{n,k}(r) = (u_{n,-k}(r))^*$

Time reversal invariant

$T\, u_{n,k}(r) = e^{i\phi(k)}\, u_{n,k}(r)$

$(u_{n,-k}(r))^* = \boxed{e^{i\phi(k)} u_{n,k}(r)}$

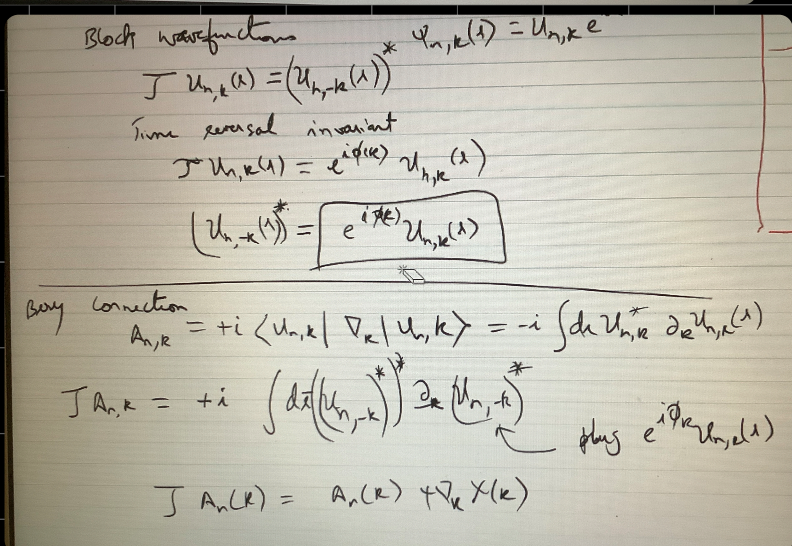
T $\quad \Omega(k) = -\Omega(-k)$

I $\quad \Omega(k) = \Omega(-k)$

$\Omega(k) = 0$

$C \neq 0$
only when
T reversal is broken

Berry connection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Berry connection

$A_{n,k} = +i\langle u_{n,k} | \nabla_k | u_{n,k}\rangle = -i\int dr\, u^*_{n,k}\, \partial_k u_{n,k}(r)$

$T A_{n,k} = +i \int d\bar{r} \left(\left(u_{n,-k}\right)^*\right)^* \partial_k \left(u_{n,-k}\right)^*$ ← plug $e^{i\phi_k} u_{n,k}(r)$

$T A_n(k) = A_n(k) + \nabla_k \chi(k)$

∵ Berry connection isn't Gauge invariant.

Berry curvature

$$= i\varepsilon_{ij}\langle \partial_{k_i} u_{n,k} | \partial_{k_j} u_{n,k}\rangle$$

$$\uparrow$$

$$= i\varepsilon_{ij}\int \frac{\partial}{\partial k_i}\left(T(u_{n,k})\right)^* \frac{\partial}{\partial k_j}\left(T(u_{n,k})\right) dr$$

$$\downarrow$$

$$\int \frac{\partial}{\partial k_i}\left(\left(u_{n,-k}\right)^*\right)^* \frac{\partial}{\partial k_j}\left(u_{n,-k}\right)^* dr$$

$$= -i\varepsilon_{ij}\int \ldots \qquad = -\Omega(k)$$

Time reversal symmetry requires

$$\Omega(-k) = -\Omega(k)$$

The chern number

$$TC = T\frac{1}{2\pi}\iint dk\, \Omega_n(k)$$

$$= \iint dk\, -\Omega_n(-k) \qquad = -C$$

$$C = -C \Rightarrow 0$$

One needs to break time reversal symmetry

$$= -i\varepsilon_{ij}\int \ldots \qquad = -\Omega(k)$$

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One needs to break time reversal symmetry

non-zero berry curvature

$\downarrow$

break TRS / IR

non-zero Chern # $\Rightarrow$ break TRS
(e.g. QHall system)

$\therefore$ reason why we could ignore BC was IR + TRS

Hashing out renewed Bloch equation derivation

$$H_{solid} = \frac{P^2}{2m} + V(\vec{r})$$

we add $\vec{E} = -\partial_t \vec{A}$ with a weak electric field.

$\downarrow$

$\vec{A}$ is spatially

[can assume const. s.t.

uniform

for x 3.7. $\nabla\phi = \vec{E}$

$$\therefore \mathcal{H} = \frac{1}{2m}(\vec{p}+e\vec{A})^2 + V(\vec{r})$$

since lattice translational invariance is still preserved, we have

$$\vec{p} = \hbar\vec{q}$$

$$H(\vec{q};t) = \frac{1}{2m}(\hbar\vec{q}+e\vec{A})^2 + V(\vec{r})$$

where $V(\vec{r})$ is a lattice transl. inv potential

short note
$\vec{\Pi} = \vec{p} - q\vec{A}$
is eqval to $m\vec{v}$,
physically measurable and hence gauge invariant.

$\therefore$ Gauge invariant crystal momenta reads

$$\vec{k} = \vec{q} + \frac{e}{\hbar}\vec{A}$$

$\because \vec{q}$ is a Good QNo. (& not $\vec{k}$),

$$\frac{d\vec{q}}{dt} = \frac{d\vec{k}}{dt} + \frac{e}{\hbar}\vec{E} = 0 \Rightarrow \frac{d\vec{k}}{dt} = \frac{-e\vec{E}}{\hbar}$$

$$\& \quad \vec{v} = \frac{d\vec{r}}{dt} = i[H,\vec{r}] = i\left[\frac{p^2}{2m},\vec{r}\right] + \frac{2i}{2m}[\vec{A}\cdot\vec{p},\vec{r}]$$

$$= \frac{i}{2m} -i\hbar\vec{p}\times 2 + \frac{2ie}{2m}\vec{A}(-i\hbar)$$

$$\vec{v} = \frac{\hbar\vec{P}}{m} + \frac{e\vec{A}}{m} = \frac{\hbar\vec{p}+e\vec{A}}{m}$$

$$\therefore \vec{v}(\vec{q}) = \frac{\hbar\vec{q}+e\vec{A}}{m} \Rightarrow \vec{v}(\vec{q}) = \frac{1}{\hbar}\nabla_{\vec{q}} H(\vec{q},t)$$

$$\vec{v}^{o}(\vec{q}) = \frac{\hbar\vec{q}+e\vec{A}(t)}{m}$$

now $H = \frac{(\vec{p}+e\vec{A})^2}{2m} + V(r)$ is a time dependent problem.

$\therefore$ net solution is

$$|\psi(x,t)\rangle = \sum_n \exp\left[\frac{-i}{\hbar}\int_{t_0}^{t} dt' E_n(t')\right] a_n(t) \, |u_n(t)\rangle$$

where $|u_n(t)\rangle$ is instantaneous eigenstate. & a_n's obey

$$i\frac{\partial\psi}{\partial t} = \mathcal{H}|\psi\rangle = \sum_n E_n(t) \, e^{\left[-i/\hbar \int_{t_0}^{t} dt' E_n(t')\right]} a_n(t)\, |u_n(t)\rangle$$

$$\Rightarrow \sum_n i\frac{da_n}{dt} e^{\frac{-i}{\hbar}(\;)} |u_n\rangle + \sum_n e^{-i(\;)} a_n \, \partial_t |u_n\rangle = 0$$

$$\Rightarrow \quad \frac{da_n}{dt} = -\sum_m \exp\left[i\int_0^{t} \omega_{nm}(t')\, dt'\right] \langle u_n(t) | \partial_t u_m\rangle$$

$$\omega_{nm} = \left[\frac{E_n - E_m}{\hbar}\right](t')$$

$$\langle u_n | \partial_t u_m\rangle = \langle u_n(\vec{R}) | \partial_t u_m(\vec{R})\rangle$$

$$= \vec{\dot{R}} \cdot \langle u_n(\vec{R}) | \nabla_R u_m(\vec{R})\rangle$$

$\hookrightarrow$ as $\vec{\dot{R}} \longrightarrow 0$, RHS $\longrightarrow 0$

content of adiabatic theorem $\Longleftarrow$ $\therefore$ state gets pinned to the evolution of initial state for small $\dot{\vec{R}}$, let $a_n(0) = 1$ & $a_m(0) = 0$.

$$\hat{\vec{v}} = \frac{d\vec{r}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{\vec{r}}]$$

But $\langle u_{mk} | e^{-ikr} \hat{\vec{v}} e^{ikr} | u_{nk} \rangle = \langle u_{mk} | \hat{v}_k | u_{nk} \rangle$

where $$\hat{v}(\vec{k}) = e^{-i\vec{k}\cdot\vec{r}} \frac{i}{\hbar}[H, \vec{r}] e^{i\vec{k}\cdot\vec{r}}$$

$$= e^{-ikr} \frac{i}{\hbar}[\hat{H}(\vec{r}, \vec{p}), \hat{r}] e^{ikr}$$

$$= \frac{i}{\hbar}[e^{-ikr} \hat{H} e^{ikr}, \hat{r}]$$

$$= \frac{i}{\hbar}[\hat{H}_k, \hat{r}]$$ where $\hat{H}_k = e^{-ikr} \hat{H}(\hat{r}, \hat{p}) e^{ikr}$

$= \hat{H}(\hat{r}, \hbar k)$

$$\Rightarrow \hat{v}_k = \frac{i}{\hbar}[\hat{H}_k, \hat{r}]$$

in momentum space $(\because \hat{r} = i\nabla_{\vec{p}})$

$$\hat{v}_k = \frac{i}{\hbar}[H_k, \hat{r}]$$

now $$\nabla_k H_k = \nabla_k e^{-i\vec{k}\cdot\hat{r}} H e^{i\vec{k}\cdot\hat{r}}$$

$$= i e^{-i\vec{k}\cdot\hat{r}} (-\hat{r} H + H \hat{r}) e^{i\vec{k}\cdot\hat{r}}$$

$$= i[\hat{H}_k, \hat{r}]$$

$$\therefore \hat{v}_k = \frac{\nabla_k H_{\vec{k}}}{\hbar}$$