Review :- ① Confined geometry tBM

↓

Gave us a wavefunction / eigenvalues.

Berry Phase :- Geometric phase ($\exists$ a variety of them)

↳ was done in context of optics

⇓

diff fields were rattling with these concepts

→ in '80s theoretical ideas converged (by M. Berry)

other phase :- Zak phase

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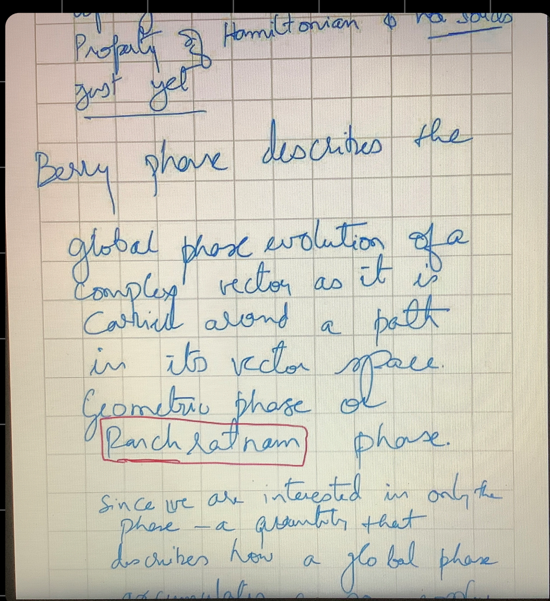

Property of Hamiltonian & its solutions just yet

Berry phase describes the global phase evolution of a complex vector as it is carried around a path in its vector space. Geometric phase or Pancharatnam phase.

Since we are interested in only the phase — a quantity that describes how a global phase

- If we adiabatically evolve the $H(\lambda)$ as a function of $\lambda(t)$. & we come back to the same point.
- If we do this adiabatic evolution, we can pick up a phase modulo 2π.

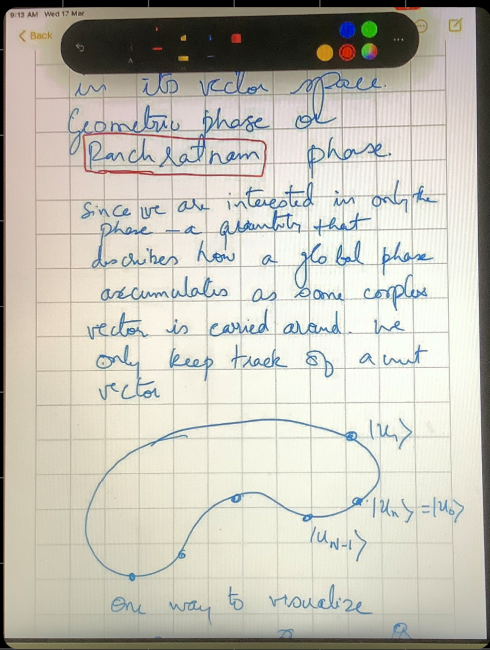
But how does Berry phase gets connected?

↳ while e^- / system evolves in real space

↓

can be mapped to evolution under k-space

now if the electron band has some Berry phase, then it can have a phase.


in its vector space.
Geometric phase or
Pancharatnam phase.

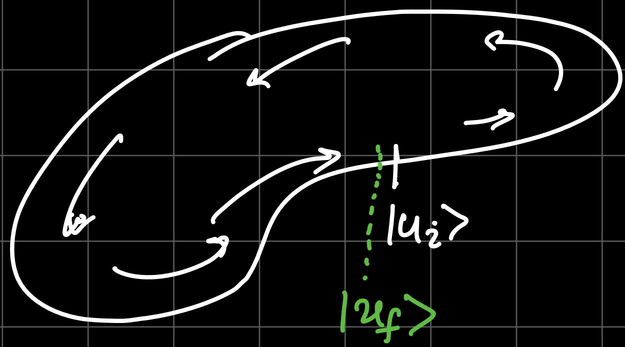
Since we are interested in only the phase — a quantity that describes how a global phase accumulates as some complex vector is carried around. We only keep track of a unit vector

$|u_1\rangle$

$|u_n\rangle = |u_0\rangle$

$|u_{N-1}\rangle$

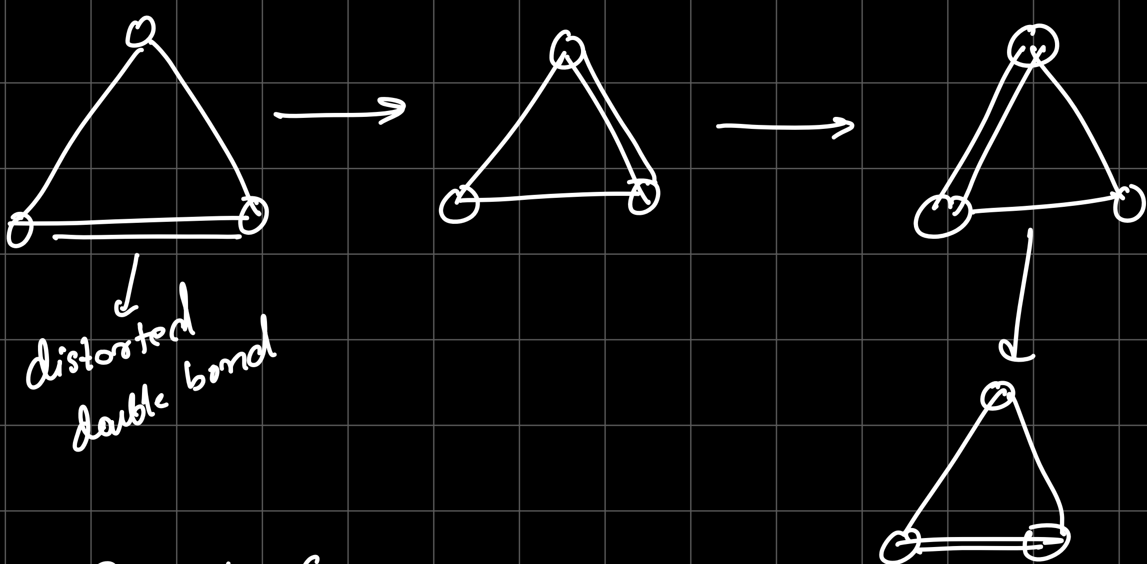
One way to visualize



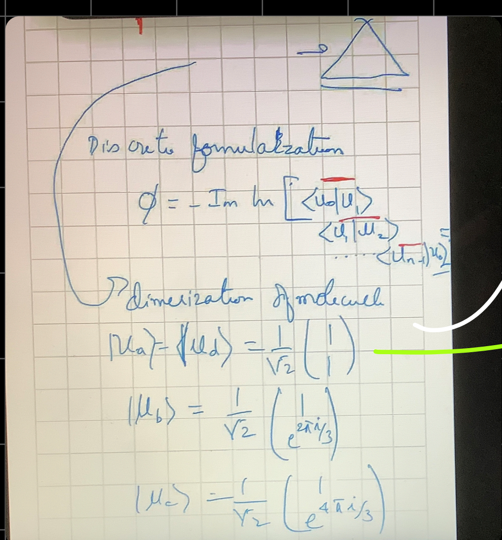
phase accumulated is $\langle u_f | u_i \rangle$

we'll often discretize this problem.

Visualization :-



Discrete formulation :-


Discrete formulization

$$\phi = -\operatorname{Im} \ln \left[\langle u_0 | u_1 \rangle \langle u_1 | u_2 \rangle \cdots \langle u_{n-1} | u_0 \rangle \right]$$

dimerization of molecule

$$|u_a\rangle = |u_d\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|u_b\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{2\pi i/3} \end{pmatrix}$$

$$|u_c\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{4\pi i/3} \end{pmatrix}$$

① David Vanderbilt's book

② @ Shen's book

two degenerate states of the triangular molecule.

$$\ln \langle u_\lambda | u_{\lambda + d\lambda} \rangle = \ln\left(1 + d\lambda \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle\right)$$

$$\approx d\lambda \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle$$

$$\approx d\lambda \langle u_\lambda | d_\lambda u_\lambda \rangle$$

$$\phi_{berry} = -\operatorname{Im} \oint \underbrace{\langle u_\lambda | d_\lambda u_\lambda \rangle d\lambda}_{\text{"purely imaginary"}}$$

system independent

$$\underline{\langle u_\lambda d_\lambda | u_\lambda \rangle + \langle u_\lambda | d_\lambda u_\lambda \rangle} = 0$$

$$\therefore \phi_{berry} = \oint \langle u_\lambda | i d_\lambda u_\lambda \rangle d\lambda$$

numerical calculation → can be done very easily.

$$A(\lambda) = \langle u_\lambda | i d_\lambda u_\lambda \rangle$$

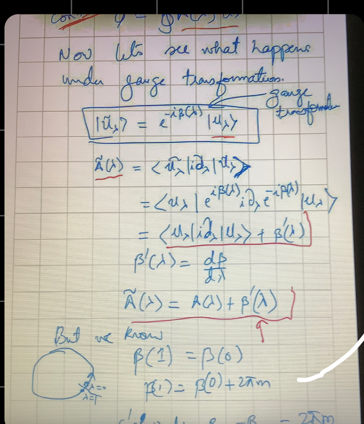
$$= -\operatorname{Im} \underline{\underline{\langle u_\lambda | d_\lambda u_\lambda \rangle}}$$

@MD → this is similar to A Bohm phase

Berry connection

$$\phi_{Berry} = \oint A(\lambda) d\lambda$$

Now see what happens under Gauge transformation:


Now lets see what happens under gauge transformation.

gauge transformation

$$\boxed{|\tilde{u}_\lambda\rangle = e^{-i\beta(\lambda)} |u_\lambda\rangle}$$

$$\tilde{A}(\lambda) = \langle \tilde{u}_\lambda | i\partial_\lambda | \tilde{u}_\lambda \rangle$$

$$= \langle u_\lambda | e^{i\beta(\lambda)} i\partial_\lambda e^{-i\beta(\lambda)} | u_\lambda \rangle$$

$$= \langle u_\lambda | i\partial_\lambda | u_\lambda \rangle + \beta'(\lambda)$$

$$\beta'(\lambda) = \frac{d\beta}{d\lambda}$$

$$\tilde{A}(\lambda) = A(\lambda) + \beta'(\lambda)$$

But we know

$$\beta(1) = \beta(0)$$

$$\beta(1) = \beta(0) + 2\pi m$$

$$\int \beta'(\lambda) d\lambda = \beta_{\lambda=1} - \beta_{\lambda=0} = 2\pi m$$

$$\Rightarrow \phi' = \phi + 2\pi m$$

$\therefore$ Berry phase is unique modulo $\underline{\underline{2\pi}}$.

Another approach with knowledge of Hamiltonian $R(t)$

$$H(R)|n(R)\rangle = E_n(R)|n(R)\rangle$$

adiabatic path along C
↳ defined by the time scale of evolution $\boxed{\tau_{ev} > \frac{\hbar}{\Delta E}}$

instantaneous eigenstate of $H(R(t))$

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

$$\sim |\psi(t)\rangle = e^{-i\theta(t)}|n(R(t))\rangle$$

$T_{evolution}$

↪ avoid crossing of levels

not enforcing this will mess things up.

not adiabatic will messup/scrambles energy levels

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

$$|\psi(t)\rangle = e^{-i\theta(t)}|n(R(t))\rangle$$

$$E_n R(t)|n(R(t))\rangle = \hbar \frac{d}{dt}\theta(t)|n(R(t))\rangle + i\hbar \frac{d}{dt}|n(R(t))\rangle$$

taking the scalar product with $\langle n(R(t))|$ and assuming $\langle n(R(t))|n(R(t))\rangle = 1$

$$E_n R(t) - i\hbar\langle n(R(t))|\frac{d}{dt}|n(R(t))\rangle = \hbar\frac{d}{dt}\theta(t)$$

$$\theta(t) = \underbrace{\frac{1}{\hbar}\int_0^t E\,R(t')\,dt'}_{\text{conventional dynamical phase}} - i\int_0^t \langle n(R(t'))|\frac{d}{dt'}|n(R(t'))\rangle\, dt'$$

Berry phase

The negative of the second part is Berry phase

$$\psi(t) = \exp\left(-\frac{i}{\hbar}\int_0^t E_n(R(t'))dt'\right)e^{i\gamma_n}|n(R(t))\rangle$$

$$\gamma_n = i\int_0^t \langle n(R(t'))|\frac{d}{dt'}|n(R(t'))\rangle\, dt'$$

this just parametrized in t

$$\gamma_n = i\int_0^{T_{cycle}} \langle n(R(t'))|\nabla_R|n(R(t'))\rangle\frac{dR}{dt'}\,dt'$$

$$= i\oint_C \langle n(R)|\nabla_R|n(R)\rangle\, dR$$

$$A_n(R) = i\langle n(R)|\frac{\partial}{\partial R}|n(R)\rangle$$

$$\gamma_n = \oint_C dR\cdot A_n(R)$$

$$\gamma_n = -\mathrm{Im}\oint\langle n(R)|\nabla_R|n(R)\rangle\, dR$$

$$A_n(R) = i\langle n(R)|\frac{\partial}{\partial R}|n(R)\rangle$$

$$\gamma_n = \oint_C dR\cdot A_n(R)$$

$$\gamma_n = -\mathrm{Im}\oint\langle n(R)|\nabla_R|n(R)\rangle\, dR$$

Using Stokes theorem

$$\gamma_n = -\mathrm{Im}\int ds\cdot\left(\nabla\times\langle n(R)|\nabla|n(R)\rangle\right)$$

$$= -\mathrm{Im}\int ds_i\,\varepsilon_{ijk}\nabla_j\langle n(R)|\nabla_k|n(R)\rangle$$

$$= -\mathrm{Im}\int ds\cdot\left(\langle\nabla n(R)|\times|\nabla n(R)\rangle\right)$$

This form is derivatives of eigenstate. One can write them as gradient

∴ Berry phase is the flux that you capture as a result of this berry capture.

the rise of 2 hamiltonians → reasons why it's best to be an optimist here.

$$= -\mathrm{Im} \int ds \cdot \left(\langle \nabla n(R) | \times | \nabla n(R) \rangle \right)$$

This form is derivatives of eigenstates
One can't write them as gradient
of Hamiltonian

$$\boxed{\varepsilon_{ijk} \langle \nabla_j (n(R)) | \nabla_k | n(R) \rangle}$$ imag

$$= \varepsilon_{ijk} \langle \nabla_j n(R) | n \rangle \langle n | \nabla_k | n(R) \rangle$$

$$+ \sum_{m \neq n} \varepsilon_{ijk} \langle \nabla_j n(R) | m \rangle \langle m | \nabla_k n(R) \rangle$$

imag

~~total~~ term `and`

$$\varepsilon_{ijk} = -\mathrm{Im} \iint ds_i \sum_{m \neq n} \langle \nabla_j n(R) | m \rangle \langle m | \nabla_k | n(R) \rangle$$

$$E_n \langle m | \nabla n \rangle = \langle m | \nabla (H n) \rangle$$

$$= \langle n | (\nabla H) | n \rangle$$

$$+ E_m \langle m | \nabla n \rangle$$

$$\boxed{\langle m | \nabla n \rangle} = \frac{\langle m | (\nabla H) | n \rangle}{(E_n - E_m)}$$

$$\Omega_n = -\iint_c ds \cdot V_n$$

evaluate gradient in hamiltonian itself.

$$+ E_m \langle m | \nabla n \rangle$$

$$\boxed{\langle m | \nabla n \rangle} = \frac{\langle m | (\nabla H) | n \rangle}{(E_n - E_m)}$$

$$\Omega_n = -\iint_c ds \cdot V_n$$

$$= -\iint_c d_s \cdot \mathrm{Im} \sum_{\boxed{m \neq n}} \frac{\langle n(R) | (\nabla_R H) | m(R) \rangle \times \langle m(R) | (\nabla_R H) | n(R) \rangle}{\left(E_n(R) - E_m(R) \right)^2}$$

Q. Why Berry curvature is a property of a system?
not of just one band?

and the identity

$$\langle u_m(\mathbf{R}) | \nabla_{\mathbf{R}} | u_n(\mathbf{R}) \rangle = \frac{\langle u_m(\mathbf{R}) | \nabla_{\mathbf{R}} H(\mathbf{R}) | u_n(\mathbf{R}) \rangle}{E_n - E_m} \qquad (4.17)$$

($m \neq n$), the Berry curvature has an alternative expression:

$$\Omega^n = Im \sum_{m \neq n} \frac{\langle u_n(\mathbf{R}) | \nabla_{\mathbf{R}} H(\mathbf{R}) | u_m(\mathbf{R}) \rangle \times \langle u_m(\mathbf{R}) | \nabla_{\mathbf{R}} H(\mathbf{R}) | u_n(\mathbf{R}) \rangle}{(E_n - E_m)^2}. \qquad (4.18)$$

It is noted that the Berry curvature in (4.15) is expressed in term of one state $u_n(\mathbf{R})$, but that in (4.18) is expressed as a summation over all possible states. It reflects that the Berry curvature describes the global properties of a system, NOT the property of a single band.

$$\vec{B} = i\,\nabla\times\left[\langle u|\nabla|u\rangle\right] = i\,\langle\nabla u|\times|\nabla u\rangle$$

$$= i\sum_n \langle\nabla u|n\rangle\times\langle n|\nabla u\rangle$$

we do it for $u \equiv$ some mth band

$$\vec{B} = i\sum_n \langle\nabla m|n\rangle\times\langle n|\nabla m\rangle$$

now $n = m$, $\langle\nabla m|m\rangle + \langle m|\nabla m\rangle = 0$

$$\Rightarrow \langle\nabla m|m\rangle\times\langle m|\nabla m\rangle = 0$$

$$\therefore\ \vec{B} = i\sum_{n\neq m}\langle\nabla m|n\rangle\times\langle n|\nabla m\rangle \quad -①$$

$$\langle n|\nabla H|m\rangle = \langle n|\nabla H|m\rangle + E_m\langle n|\nabla|m\rangle$$

$$\Rightarrow \underset{m\neq n}{E_n}\langle n|\nabla m\rangle = \langle n|\nabla H|m\rangle + E_m\langle n|\nabla m\rangle$$

$$\Rightarrow \langle n|\nabla m\rangle = \frac{\langle n|\nabla H|m\rangle}{E_n - E_m} = -\frac{\langle n|\nabla H|m\rangle}{E_m - E_n} \quad -②$$

$$\Rightarrow \langle\nabla m|n\rangle = -\frac{\langle m|\nabla H|n\rangle}{E_m - E_n} =$$

Put ② in ① to get

$$\vec{B} = i\sum_n \frac{\langle m|\nabla H|n\rangle}{E_m - E_n}\times -\frac{\langle n|\nabla H|m\rangle}{E_n - E_m}$$

$$\vec{B} = \sum_n i\,\frac{\langle m|\nabla H|n\rangle\times\langle n|\nabla H|m\rangle}{(E_m - E_n)^2}$$

or $$\vec{\Omega}_n = \sum_{m\neq n} \frac{i\,\langle m|\nabla H|n\rangle\times\langle n|\nabla H|m\rangle}{(E_m - E_n)^2}$$

$$\therefore \quad \underline{\underline{\sum_n \vec{\Omega}_n = 0}}$$