Berry phase

Geometry and topology in quantum mechanics give B.P.

It is based on adiabatic evolution of Hamiltonian $H(\lambda)$, where λ is some external parameter, like position of atoms in the unit cell or external field.

If we change λ slowly enough, we can derive how the eigenstates change with λ, provided that:

- the states are non-degenerate (unique)

  [Can be exact many-body eigenstates, not just single particle states]

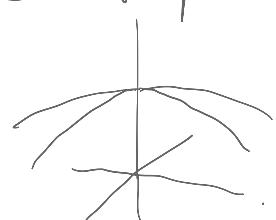
  [If degeneracy is known (p) we can generalize the concept to arbitrary p, but this will give rise to different quantum (instead of $2\pi M \to 2\pi p \cdot M$)]

  integer Q.H.F $\to$ fractional Q.H.F

- the parameter λ is varied slowly enough

  It has to be slow enough so that the system is never excited to the neighboring state. this means that there has to be a gap in the excitation spectrum. This is therefore not valid for metals.

In electronic structure there is a lot of level crossings at high symmetry points:



To take care of such situation we need to treat the group of bands as a common unit and arrange a "smooth gauge" through the crossings.

We vary parameter λ in $H(\lambda)$ but eventually we go back to the initial state (like $z=0 \dots 2\pi$ in BZ, and 2π is the same point as 0)

If we go around in the phase space $\lambda_0 \to \lambda_1 \to \lambda_2 \dots \to \lambda_N = \lambda_0$, we must arrive to the same wave function, but only up to a phase

$$|\psi\rangle \to e^{i\gamma} |\psi\rangle \quad \text{(geometric part of } \gamma \text{ is Berry phase)}$$

γ is important when we look at interference effects.

If adiabatic theorem is satisfied! $H(\lambda)\,|m(\lambda)\rangle = E_m(\lambda)\,|m(\lambda)\rangle$

the state of the system is parametrized by the ansatz $|\psi(t)\rangle = \underbrace{C(t)}_{\text{extra phase}} \underbrace{e^{-i\int_0^t E_m(t')dt'}}_{U} |m(t)\rangle$

S.E. satisfied at each time: $\left(i\frac{\partial}{\partial t} - H\right)|\psi(t)\rangle = 0$

remember $|m\rangle = |m(t)\rangle$ and $C(t)$ and $E_m(t)$, ---

$$i\left(\dot{C}\,U\,|m\rangle - i E_m(t)\, C\,U\,|m\rangle + C\,U\,|\tfrac{dm}{dt}\rangle\right) - H\,\underbrace{C\,U}_{\text{numbers}}\,|m\rangle = 0$$

$$i\,\dot{C}\,U|m\rangle + E_m(t)\,C\,U|m\rangle + i\,C\,U\,|\tfrac{dm}{dt}\rangle - C\,U\,E_m|m\rangle = 0$$

$$\langle m| \;/\; \dot{C}\,|m\rangle + C\,|\tfrac{dm}{dt}\rangle = 0$$

$$\dot{C} + C\langle m|\tfrac{dm}{dt}\rangle = 0 \implies C = e^{i\phi(t)} = e^{-\int_0^t \langle m(t')|\frac{\partial m}{\partial t'}\rangle dt'}$$

with $\phi(t) = i\int_0^t \langle m(t')|\frac{\partial m(t')}{\partial t'}\rangle dt'$

but $|m(t)\rangle = |m(\lambda(t))\rangle$ hence

$$|\tfrac{\partial m}{\partial t}\rangle = |\tfrac{\partial m}{\partial \lambda}\rangle \frac{d\lambda}{dt} \quad \text{and} \quad \langle m(t')|\tfrac{\partial m(t')}{\partial t'}\rangle = \langle m(\lambda)|\tfrac{\partial m}{\partial \lambda}\rangle \dot{\lambda}$$

Hence

$$\phi(t) = i\int_{\lambda(0)}^{\lambda(t)} \langle m(\lambda)|\tfrac{\partial m}{\partial \lambda}\rangle\, d\lambda$$

ϕ depends only on λ and not on type of time evolution (details of t. evolution)

We conclude that $|\psi(t)\rangle = e^{i\phi(\lambda(t))}\, e^{-i\int_0^t E_m(t')dt'}\, |m(t)\rangle$

If $\lambda_{final} = \lambda(0)$ then $\phi = i \oint \langle M(\lambda) | \frac{\partial M}{\partial \lambda} \rangle \, d\lambda$

where adiabatic evolution gives: $|\psi(t)\rangle = e^{i\phi(\lambda(t))} \, e^{-i\int_0^t E_n(t')\,dt'} \, |M(t)\rangle$

Again define Berry connection: $A^\mu(\lambda) = \langle M(\lambda) | i \frac{\partial M(\lambda)}{\partial \lambda_\mu} \rangle$

Berry phase: $\phi = \sum_\mu \int d\lambda_\mu \, A^\mu(\lambda)$ (like $\oint \vec{A} \cdot d\vec{l}$)

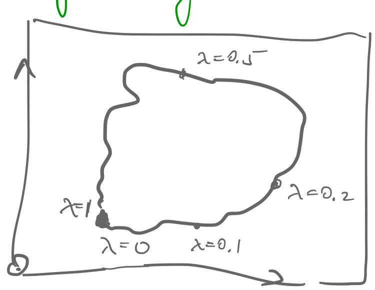
Berry curvature: $\Omega^{\mu\nu} = \left(\frac{\partial}{\partial \mu} A^\nu(\lambda) - \frac{\partial}{\partial \nu} A^\mu(\lambda) \right)$ (like $\vec{\nabla} \times \vec{A}$)

Note: $\Omega^{\mu\nu} = i \left[\frac{\partial}{\partial \lambda_\mu} \left(\langle M | \frac{\partial}{\partial \lambda_\nu} M \rangle \right) - \frac{\partial}{\partial \lambda_\nu} \left(\langle M | \frac{\partial}{\partial \lambda_\mu} M \rangle \right) \right]$

$$= i \left(\langle \frac{\partial M}{\partial \lambda_\mu} | \frac{\partial M}{\partial \lambda_\nu} \rangle - \langle \frac{\partial M}{\partial \lambda_\nu} | \frac{\partial M}{\partial \lambda_\mu} \rangle \right)$$

$$\Omega^{\mu\nu} = -2 \, \mathrm{Im} \langle \frac{\partial M}{\partial \lambda_\mu} | \frac{\partial M}{\partial \lambda_\nu} \rangle$$

Gauge transformation is freedom in choosing initial $|M(\lambda_0)\rangle$. We could choose $|\tilde{M}(\lambda_0)\rangle = e^{-i\beta(\lambda)} |M(\lambda_0)\rangle$ and require that $\beta(\lambda=1) - \beta(\lambda=0) = 2\pi M$ when $\lambda_f = \lambda_i$ and the system goes around a closed loop



Then $\tilde{A}^\mu(\lambda) = A^\mu(\lambda) + \frac{d\beta}{d\lambda_\mu}$ $\vec{A}$ is not gauge invariant (like potential $\vec{A}$)

$\tilde{\phi} = \oint \tilde{A}(\lambda)\, d\lambda + \beta(\lambda=1) - \beta(\lambda=0) = \phi + 2\pi M$ ϕ is unique up to a quantum

$\tilde{\Omega}^{\mu\nu} = \frac{\partial \tilde{A}^\nu}{\partial \lambda_\mu} - \frac{\partial \tilde{A}^\mu}{\partial \lambda_\nu} = \Omega^{\mu\nu} + \underbrace{\frac{d^2\beta}{d\lambda_\mu \partial \lambda_\nu} - \frac{d^2\beta}{d\lambda_\nu d\lambda_\mu}}_{=0} = \Omega^{\mu\nu}$ Ω is gauge invariant and unique.

(like magnetic field B)

Cern theorem says:

$$\frac{1}{2\pi}\iint \Omega^{\mu\nu}\, d\lambda_\mu\, d\lambda_\nu = C \in \text{Integer}$$

Consider 2D space λ_1 and λ_2.

We see that $\phi = \int dx_1\, A^1(x) + \int dx_2\, A^2(x)$

and then $\Omega^{12} = \frac{\partial}{\partial x_1} A^2 - \frac{\partial}{\partial x_2} A^1 = (\vec{\nabla}\times\vec{A})_3$

Stokes theorem says $\int \Omega^{12}\, dx_1\, d\lambda_2 = \int (\vec{\nabla}\times\vec{A})_3\, d\lambda_1 d\lambda_2 = \oint \vec{A}\cdot d\vec{l} = \phi(f) - \phi(i) = 2\pi C$

closed path

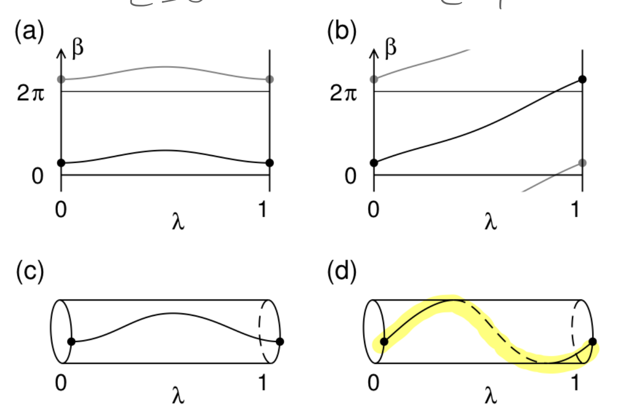
but this is the same state, hence $2\pi C$

Other forms of Chern theorem:

$$-2\iint \text{Im}\left\langle \frac{\partial u}{\partial \lambda_\mu} \middle| \frac{\partial u}{\partial \lambda_\nu}\right\rangle d\lambda_\mu\, d\lambda_\nu = 2\pi C$$

What can happen to ϕ?

C=0 C=1



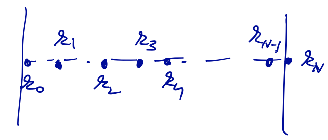
periodic boundary condition in λ-space

Figure 3.5 Possible behaviors of the function $\beta(\lambda)$ defining a gauge transformation through Eq. (3.15). (a-b) Conventional plots of "progressive" (a) and "radical" (b) gauge transformations, for which β returns to itself or is shifted by a multiple of 2π at the end of the loop, respectively. Shaded lines show 2π-shifted periodic images. (c-d) Same as (a-b) but plotted on the surface of a cylinder to emphasize the nontrivial winding of the radical gauge transformation in (b) and (d).

<u>Practical calculations</u> use formula:

$$\Phi = -\operatorname{Im} \ln\left(\langle u_{\lambda_0} | u_{\lambda_1}\rangle \langle u_{\lambda_1} | u_{\lambda_2}\rangle \cdots \langle u_{\lambda_{N-1}} | u_{\lambda_N}\rangle\right)$$

λ for k-space



but $|u_{\lambda_N}\rangle$ in closed loop is $e^{i2\pi m} |u_{\lambda_0}\rangle$

$$\Phi = -\operatorname{Im} \ln\left(\langle u_{\lambda_0} | u_{\lambda_1}\rangle \langle u_{\lambda_1} | u_{\lambda_2}\rangle \cdots \langle u_{\lambda_{N-1}} | u_{\lambda_0}\rangle\right)$$

Why is this the same?

$$\langle u_\lambda | u_{\lambda+\delta\lambda}\rangle = \langle u_\lambda | u_\lambda + \frac{\partial u_\lambda}{\partial \lambda}\delta\lambda + \cdots\rangle = 1 + \langle u_\lambda | \frac{\partial u}{\partial\lambda}\rangle \delta\lambda$$

$$\ln \langle u_\lambda | u_{\lambda+\delta\lambda}\rangle \approx \ln\left(1 + \delta\lambda \langle u_\lambda | \frac{\partial u}{\partial \lambda}\rangle\right) \approx \boxed{\langle u | \frac{\partial u}{\partial\lambda}\rangle \delta\lambda}$$

Note that: $2\operatorname{Re}\langle u | \frac{\partial u}{\partial\lambda}\rangle = \langle u | \frac{\partial u}{\partial \lambda}\rangle + \langle u | \frac{\partial u}{\partial\lambda}\rangle^* = \langle u | \frac{\partial u}{\partial\lambda}\rangle + \langle \frac{\partial u}{\partial\lambda} | u\rangle = \frac{\partial}{\partial\lambda}\langle u | u\rangle = 0$

hence $\langle u | \frac{\partial u}{\partial\lambda}\rangle$ is purely imaginary and

$$\Phi = -\operatorname{Im} \ln \prod_{i=0}^{N} \langle u_{\lambda_i} | u_{\lambda_{i+1}}\rangle = -\operatorname{Im} \int \langle u | \frac{\partial u}{\partial \lambda}\rangle d\lambda = \int i \langle u | \frac{\partial u}{\partial\lambda}\rangle d\lambda$$

Why do we use the discrete formula?

Every eigenstate $|u_{\lambda_i}\rangle$ has an arbitrary phase $|\tilde{u}_{\lambda_i}\rangle = e^{i\beta} |u_{\lambda_i}\rangle$ and using numerically determined eigenvectors $|u_{\lambda_i}\rangle$ the phase will never be a smooth function of λ. But adiabatic theorem requires smoothness. The discrete formula is gauge free, because each $|u_{\lambda_i}\rangle$ appears exactly twice, once as bra, and once as ket:

$$\Phi = -\operatorname{Im} \ln\left(\langle u_{\lambda_0} | u_{\lambda_1}\rangle \langle u_{\lambda_1} | u_{\lambda_2}\rangle \langle u_{\lambda_2} | \cdots \langle u_{\lambda_{N-1}} | u_{\lambda_0}\rangle\right)$$

simple phase $e^{i\beta_j} |u_{\lambda_j}\rangle$ cancels

We need to use u_{λ_0} rather than u_{λ_N}!

$$\cdots e^{+i\beta_j} |u_{\lambda_j}\rangle \langle u_{\lambda_j}| e^{-i\beta_j} \cdots$$

Example of Berry phase: Spin 1/2 particle in a magnetic field $\vec{B} = B\vec{n}$

where $\vec{n}$ is slowly (adiabatically) varies with time.

$$H = -\mu_B B\, \vec{n}\cdot\vec{\sigma}$$

Here x is $\vec{n}(x)$ and changes with time.

The ground state is spinor pointing in the direction of $\vec{n}$, i.e., instantaneous σ_z.

From Q.M. course we know that $|\psi_\uparrow\rangle = \begin{pmatrix}\cos\theta/2 \\ \sin\theta/2\, e^{i\varphi}\end{pmatrix}$ where (θ,φ) are determined from $\vec{n} = \begin{pmatrix}\sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta\end{pmatrix}$.

Note that when $\theta=\pi$, we have $|\psi_\uparrow\rangle = \begin{pmatrix}0 \\ e^{i\varphi}\end{pmatrix}$ and any φ will give different phase. This will make $\theta=\pi$ a special point with singularity of Ω, and consequently nontrivial Berry phase.

We can compute $\vec{A} = i\langle\psi_\uparrow|\frac{\partial\psi_\uparrow}{\partial\vec{n}}\rangle$ in spherical coordinates. We have

$$A_\theta = \langle\psi_\uparrow|\tfrac{\partial}{\partial\theta}|\psi_\uparrow\rangle = i\left(\cos\theta/2,\ \sin\theta/2\, e^{-i\varphi}\right)\cdot\frac{\partial}{\partial\theta}\begin{pmatrix}\cos\theta/2 \\ \sin\theta/2\, e^{i\varphi}\end{pmatrix} = 0$$

$$A_\varphi = \langle\psi_\uparrow|\tfrac{1}{\sin\theta}\tfrac{\partial}{\partial\varphi}|\psi_\uparrow\rangle = -\frac{\sin^2\theta/2}{\sin\theta}$$

$$\vec{\Omega} = \vec{\nabla}\times\vec{A} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(A_\varphi\sin\theta\right)\vec{e}_r + \cdots = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin^2\theta/2\right)\vec{e}_r = -\frac{1}{2}\,\frac{2\sin\theta/2\cos\theta/2}{\sin\theta}\,\vec{e}_r = -\frac{1}{2}\vec{e}_r$$

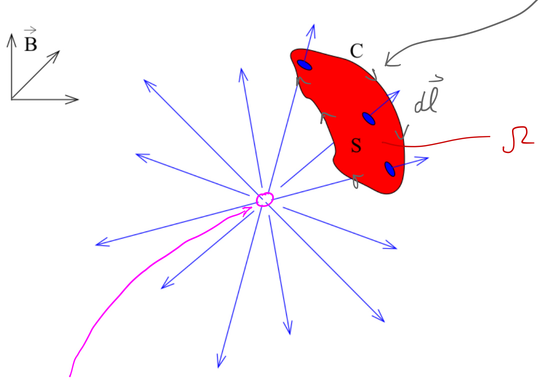
Berry curvature is constant on the sphere and looks like a magnetic monopole.

The Berry phase $\quad \Phi = \oint\vec{A}\cdot d\vec{l} = \int\vec{\Omega}\cdot\frac{d\vec{S}}{r^2} = -\frac{1}{2}\int d\Omega = -\frac{\Omega}{2}$

quarter of the sphere $\Omega = \frac{4\pi}{4}\left(-\frac{1}{2}\right) = -\frac{\pi}{4}$

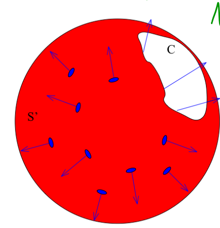
half the sphere $\Omega = -\frac{\pi}{2}$

entire sphere $\Phi = -2\pi \Rightarrow$ chern number $= -1$



Singularity of Ω gives nonzero Chern number.

We could equally well use this surface in Stokes. We would get



$$\Phi = -(4\pi-\Omega)\left(-\tfrac{1}{2}\right) = 2\pi - \frac{\Omega}{2}$$

because opposite orientation in integration

equivalent!

Example 2: We have a molecule, which goes through a sequence of transformations $(a) \to (b) \to (c) \to (d) = (a)$

See picture.

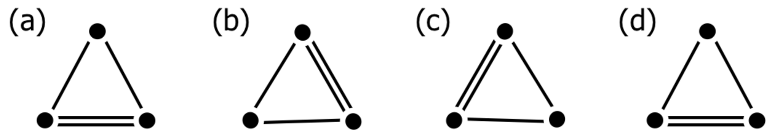


Figure 3.2 Triangular molecule going though a sequence of distortions in which first the bottom, then the upper-right, then the upper-left bond is the shortest and strongest of the three. The configurations in panels (a) and (d), representing the beginning and end of the loop, are identical.

Let's suppose that the wave functions are $u_a = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ $u_b = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{2\pi i/3} \end{pmatrix}$

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

What is Berry's phase?

The discrete formula is $\phi = -\operatorname{Im} \ln \langle u_a | u_b \rangle \langle u_b | u_c \rangle \langle u_c | u_a \rangle = -\pi$

$$\left(e^{\pi i/3} \cos\frac{\pi}{3}\right) \left(e^{\pi i/3} \cos\frac{\pi}{3}\right) \left(e^{\pi i/3} \cos\frac{\pi}{3}\right)$$

Berry phase in the Brillouine zone

Here we take $x_1 = k_x$ $x_2 = k_y$ and $x_3 = k_z$ and evolve our system through the Brillouine zone (like what we need for polarization).

$$\vec{A}_{n\vec{k}} = i \langle u_{n\vec{k}} | \frac{\partial}{\partial \vec{k}} u_{n\vec{k}} \rangle$$

$$\vec{\Omega}_{n\vec{k}} = \vec{\nabla} \times \vec{A}_{n\vec{k}}$$

$$\phi_n = \oint \vec{A}_{n\vec{k}} \cdot d\vec{k} = \int_{\text{inside the loop}} (\vec{\nabla} \times \vec{A}_{nk}) \cdot d\vec{S}_k = \int_{\text{inside the loop}} \vec{\Omega}_{nk} \cdot d\vec{S}_k$$

Note $\Omega_{n\vec{k}}$ is uniquely defined (gauge invariant) and has the following properties:

1) If the crystal has inversion symmetry I, then $\Omega(\vec{k}) = \Omega(-\vec{k})$.
2) If the crystal has time reversal symmetry (TR) then $\Omega(\vec{k}) = -\Omega(-\vec{k})$
3) If the crystal has some other symmetry, $\Omega(\vec{k})$ inherits it.

consequence If we have $I + TR \Rightarrow \Omega(\vec{k}) = 0$! No Berry phase or chern number.

(the same symmetries as $\vec{B}$ has, because is $\vec{\nabla} \times \vec{A}$).