Berry phase

① Adiabatic evolution of quantum systems

② Calculation of topological invariant.

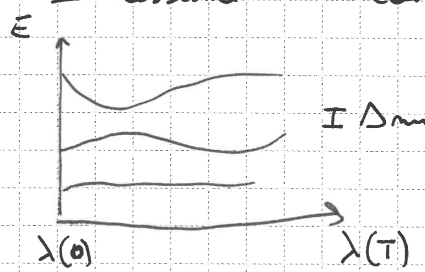
To a certain extent ② ⊂ ① ⇒ see TKNN invariant

Let us start from ①.

I consider a system evolving in time based on $H(\lambda(t))$. For each value of λ I define the istantaneous eigenbasys:

$$H(\lambda(t))\,|m(\lambda(t))\rangle = E_m(\lambda(t))\,|m(\lambda(t))\rangle$$

I assume we can apply the adiabatic theorem:



I Δ_{min} $\quad$ Δ_{min} / $T \gg \frac{1}{\Delta_{min}}$

In this situation adiabaticity tells me that

$$|\psi(t=0)\rangle = |m(\lambda(t=0))\rangle \Rightarrow |\psi(t)\rangle = e^{i\tilde{\alpha}}\,|m(\lambda(t))\rangle$$

In particular I redefine $\tilde{\alpha}$:

$$|\psi(t)\rangle = e^{-i\int_0^t E_m(t')\,dt'}\; e^{i\alpha(\lambda(t))}\;|m(\lambda(t))\rangle$$

α depends only on λ: this is what we want to show

Schrödinger Equation:

$$i\,\partial_t |\psi(t)\rangle = H(t)|\psi(t)\rangle$$

$$\Rightarrow \cancel{E_n(\lambda(t))|\psi(t)\rangle} - \partial_t\alpha(t)|\psi(t)\rangle + i\,e^{-i\int_0^t E_n(t')dt' + i\alpha(t)}|\partial_t n(\lambda(t))\rangle$$

$$= \cancel{E_n(\lambda(t))|\psi(t)\rangle}$$

$$\Rightarrow \langle\psi(t)|\,\partial_t\alpha(t)\,|\psi(t)\rangle = \langle\psi(t)|\,i\,e^{-i\int^t E_n dt' + i\alpha}|\partial_t n(\lambda(t))\rangle$$

$$\Rightarrow \partial_t\alpha(t) = i\langle n(\lambda(t))|\partial_t n(\lambda(t))\rangle =$$

$$= i\langle n(\lambda(t))|\partial_\lambda n(\lambda(t))\rangle \cdot \frac{\partial\lambda}{\partial t}$$

$$\Rightarrow \alpha(t) = \int_0^t dt'\,\frac{d\lambda}{dt'}\,i\langle n(\lambda(t'))|\partial_\lambda|n(\lambda(t'))\rangle =$$

$$= \int_{\lambda_i}^{\lambda_f} d\lambda\,\underbrace{i\langle n(\lambda)|\partial_\lambda n(\lambda)\rangle}_{A_n(\lambda)\,:\,\boxed{\text{Berry connection}}}$$

In the case of adiabatic cycle I impose:

$$\lambda_i = \lambda_f \quad \text{and} \quad |n(\lambda(0))\rangle = |n(\lambda(T))\rangle$$

$\Rightarrow$ no additional phase in the choice of this basis:

$$\Rightarrow \alpha_n = \oint d\lambda\,A_n(\lambda) \quad \Rightarrow \boxed{\text{Berry phase}}$$

It depends only on the GEOMETRY of the cycle!

The Berry phase must be independent on the basis choice.

$\Rightarrow$ Gauge transformation.

I consider a new basis:

$$|n'(t)\rangle = e^{-i\beta(t)} |n(\lambda(t))\rangle$$

$$\Rightarrow |\psi(t)\rangle = e^{-i\int_0^t E_n(t')dt' + i\alpha(\lambda(t)) + i\beta(t)} |n'(t)\rangle$$

$$\Rightarrow \alpha'(t) = \alpha(t) + \beta(t)$$

$$\Rightarrow \alpha_{Berry} = \int_{t=0}^{T} dt\, \partial_t \alpha'(t) - \int_0^T \partial_t \beta(t) =$$

$$= \underbrace{\oint d\lambda\, i\langle n'|\partial_\lambda n'\rangle}_{\text{Berry connection}} \underbrace{- \beta(T) + \beta(0)}_{\text{explicit basis tr.}}$$

If $\beta(T) \neq \beta(0)$ I must account for it!

If β depends only on λ: $\beta(\lambda(t))$

$$\Rightarrow \boxed{\beta(T) = \beta(0)} \quad \text{and} \quad \boxed{A(\lambda) = A'(\lambda) - \partial_\lambda \beta}$$

Typical example : spin 1/2 :

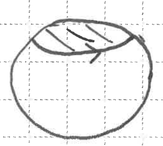
$$H = -\vec{\sigma}\cdot\vec{\lambda} \quad / \quad |\lambda| \neq 0 \Rightarrow \text{gapped}$$

$$\vec{\lambda} = |\lambda| \left(\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta \right)$$

$$\Rightarrow \quad |\psi_{GS}\rangle = \cos\frac{\theta}{2}\,|\uparrow\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|\downarrow\rangle$$

$$A_{|\lambda|} = 0 \qquad A_\theta = i \left(\cos\frac{\theta}{2} \quad e^{-i\varphi}\sin\frac{\theta}{2} \right) \frac{1}{2} \begin{pmatrix} -\sin\theta/2 \\ e^{i\varphi}\cos\frac{\theta}{2} \end{pmatrix} = 0$$

$$A_\varphi = i \sin^2\frac{\theta}{2} \cdot i = -\sin^2\frac{\theta}{2} = -\frac{1-\cos\theta}{2}$$

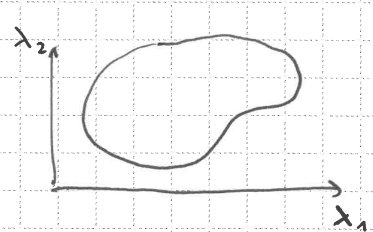


θ fixed

$$\alpha_{Berry} = \oint d\varphi\, A_\varphi = -2\pi \left(\frac{1-\cos\theta}{2} \right) =$$

$$= -\frac{1}{2}\,\Omega_{angle}$$

More in general :



Berry connection :

$$\vec{A} = i\langle n|\vec{\nabla}_\lambda n\rangle$$

Berry curvature :

$$\vec{F} = \vec{\nabla} \times \vec{A}$$

Berry phase : $\alpha = \oint \vec{A}\cdot d\vec{\lambda} = \int d^2\lambda \cdot \vec{F}$

Spin 1/2 in spherical coordinates:

$$\vec{\nabla} = \left(\partial_r , \frac{1}{r} \partial_\theta , \frac{1}{r \sin\theta} \partial_\varphi \right)$$

$$\vec{A}_\varphi = \frac{1}{|\lambda| \sin\theta} \left(- \sin^2 \frac{\theta}{2} \right) = - \frac{1}{2|\lambda|} \operatorname{tg} \frac{\theta}{2}$$

$$\vec{F}_r = \frac{1}{|\lambda| \sin\theta} \partial_\theta \left(\sin\theta \, A_\varphi \right) = - \frac{1}{2|\lambda|^2} \cancel{2} \frac{\sin\theta/2 \cos\theta/2}{\sin\theta} \frac{1}{\cancel{2}} = - \frac{1}{2|\lambda|^2}$$

$$\text{Berry phase} = \int F_r \cdot dA = - \frac{1}{2} \int \frac{\hat{R}}{R^2} \cdot dA = - \frac{1}{2} \Omega_{\text{angle}}$$

BERRYOLOGY AND CHERN NUMBER

Lattice model in 2D with 2 bands

$$H(\vec{k}) = \alpha_0 \mathbb{1} + \vec{\alpha}(\vec{k}) \cdot \vec{\sigma} \quad \rightarrow 2\times 2 \text{ Matrix}$$

α_0: does not influence the wavefunction properties

$\Rightarrow$ In clean systems does not influence topological properties

TOPOLOGY

$$\vec{k} \in BZ \xrightarrow{H_{gapped}} \lambda(\vec{k}) = \frac{\vec{\alpha}(\vec{k})}{|\vec{\alpha}(\vec{k})|} \in S^2 \longrightarrow \psi_{GS}(k) = \cos\frac{\theta}{2}|\uparrow\rangle + e^{i\varphi}\sin\frac{\theta}{2}|\downarrow\rangle$$

$\downarrow$ Torus $(0,2\pi]\times(0,2\pi]$; Sphere

Rescaling: does not influence wavefunctions

$\psi_{GS}(k)$ lives in a sphere [Bloch sphere]

We consider $|\vec{\alpha}(\vec{k})| \neq 0 \quad \forall \vec{k}$: gapped system.

$\vec{\alpha} = 0 \Rightarrow$ gapless critical point

Mapping from torus to sphere is characterized by a topological index [element of the homotopy group]:

$$C = \frac{1}{2\pi}\int_{BZ} dk \; F$$

: first Chern number: specifies homotopy mapping

Here:

$$\vec{F} = \vec{\nabla} \times \vec{A}(\vec{k}) = i\left[\langle \partial_{k_x}\psi | \partial_{k_y}\psi\rangle - \langle \partial_{k_y}\psi | \partial_{k_x}\psi\rangle\right]$$

$$\vec{A}(\vec{k}) = i\langle \psi(k) | \vec{\nabla}_k \psi(k)\rangle$$

C is an integer $\rightarrow$ Non-local order parameter

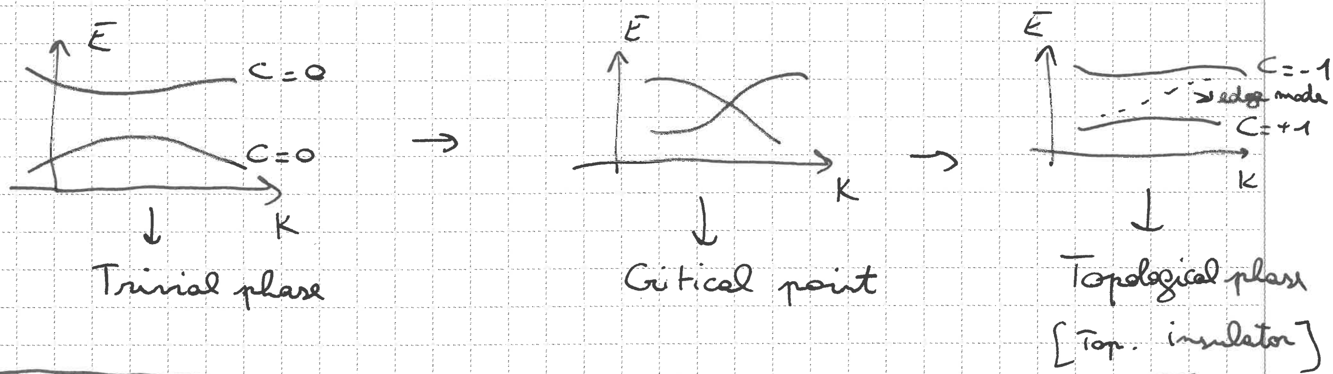
C is the Hall conductivity: KUBO:

$$\sigma = i \sum_{\alpha < E_F} \sum_{\beta > E_F} \frac{(\partial H/\partial k_x)_{\alpha\beta}(\partial H/\partial k_y)_{\beta\alpha} - (\partial H/\partial k_y)_{\alpha\beta}(\partial H/\partial k_x)_{\beta\alpha}}{(\varepsilon_\alpha - \varepsilon_\beta)^2}$$

Trick: $v_i = \frac{\partial H}{\partial k_i} = [H, x_i]$

Summarizing : C is

- Chern Number
- Flux of the Berry conductivity
- (Anomalous) Hall conductivity
- Number of chiral edge modes
- Order parameter for Topological phase transition



Symmetries :

T symmetry : $F(\vec{k}) = -F(-\vec{k}) \Rightarrow C = 0$

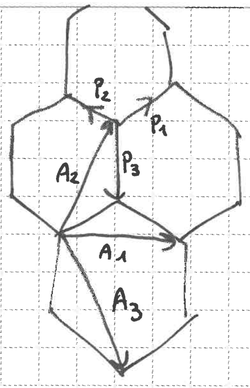
$\psi(k) \to \psi^*(-k)$

P symmetry : $F(\vec{k}) = F(-\vec{k})$

$\psi(k) \to \psi(-k)$

$\Rightarrow$ PT symmetry $\Rightarrow F = 0$!

HALDANE MODEL



$P_1 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$ $P_2 = \left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$ $P_3 = (0, -1)$

$A_1 = (\sqrt{3}, 0)$ $A_2 = \left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right)$ $A_3 = \left(\frac{\sqrt{3}}{2}, -\frac{3}{2}\right)$

$$H = \underbrace{H_{graphene} + \text{Staggering}}_{H_{NN}} + \underbrace{\text{NNN terms with flux}}_{H_{NNN}}$$

$$H_{NN} = \begin{pmatrix} \Delta & -J\sum_\gamma e^{-i\vec{k}\cdot\vec{P}_\gamma} \\ -J\sum_\gamma e^{i\vec{k}\cdot\vec{P}_\gamma} & -\Delta \end{pmatrix}$$

$$H_{NNN} = -2J' \begin{pmatrix} \sum_\gamma \cos(\vec{k}\cdot\vec{A}_\gamma - \phi) & 0 \\ 0 & \sum_\gamma \cos(\vec{k}\cdot\vec{A}_\gamma + \phi) \end{pmatrix}$$

$$H = -2J'\cos\phi \sum_\gamma \cos\vec{k}\cdot\vec{A}_\gamma \cdot \mathbb{1} - J\sum_\gamma \cos\vec{k}\cdot\vec{P}_\gamma\, \sigma_x$$
$$-J\sum_\gamma \sin\vec{k}\cdot\vec{P}_\gamma\, \sigma_y + \left(\Delta - 2J'\sin\phi \sum_\gamma \sin\vec{k}\cdot\vec{A}_\gamma\right)\sigma_z$$

Band touching points in $\vec{k} = \left(\pm\frac{2\pi}{3\sqrt{3}}, 0\right)$ for:

$$\Delta = \pm 3J'\sqrt{3}\sin\phi$$