

## Leet 6: Topological index for quantum Hall system

Magnetic translation for  $H = \frac{(\vec{P} - \frac{e}{c}\vec{A})^2}{2m}$  with  $\nabla \times \vec{A} = B\hat{z}$

① symmetric gauge  $\vec{A} = \frac{B}{2}\hat{z} \times \vec{r} = \frac{B}{2}(-y, x)$

$$T_x = e^{-i\delta_x \cdot (P_x + \frac{e}{c}A_x)/\hbar} = e^{-i\delta_x [-i\hbar\partial_x - \frac{eB}{2c}y]/\hbar}$$

$$T_y = e^{-i\delta_y (P_y + \frac{e}{c}A_y)/\hbar} = e^{-i\delta_y (-i\hbar\partial_y + \frac{eB}{2c}x)/\hbar}$$

② Landau gauge  $\vec{A} = -B(y, 0)$

$$T_x = e^{-i\delta_x P_x/\hbar} \quad T_y = e^{-i\delta_y [P_y + \frac{eB}{c}x]/\hbar}$$

Please check that  $[T_x, H] = [T_y, H] = 0$ . for these two gauges.

Magnetic Bloch theorem:

Define a magnetic unit cell with  $L_x \times L_y$  which encloses a fundamental flux  $\Phi_0$ . Then

$$\psi_{k_x, k_y}(x, y) = e^{ik_x x + ik_y y} u_{k_x, k_y}(x, y)$$

with  $u_{k_x, k_y}(x+L_x, y) = e^{i2\pi L_x A_x / \Phi_0} u_{k_x, k_y}(x, y)$

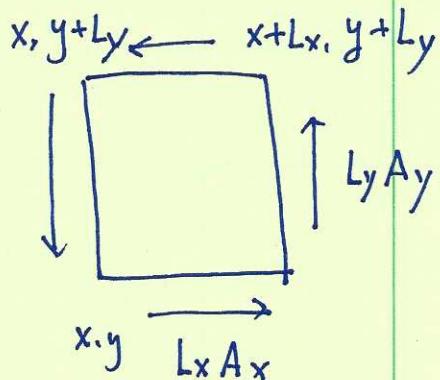
$$u_{k_x, k_y}(x, y+L_y) = e^{i2\pi L_y A_y / \Phi_0} u_{k_x, k_y}(x, y)$$

for the symmetric gauge.

HW: write down the magnetic Bloch theorem for the Landau gauge.

Define:

$$u_{k_1 k_2}(x, y) = |u_{k_1 k_2}(x, y)| e^{i \Theta_{k_1 k_2}(x, y)}$$



winding number

$$P = \frac{+1}{2\pi} \oint d\vec{l} \cdot \nabla_l \Theta_{k_1 k_2}$$

— the number of zeros of  $u_{k_1 k_2}$ , i.e., vorticity.

$$\oint d\vec{l} \cdot \nabla_l \Theta_{k_1 k_2} = 2\pi \Phi_0 / \Phi_0 = 2\pi \Rightarrow P = 1.$$

HW: ① Verify that  $P$  is gauge-independent.

② Consider solving the B-deG equation for superconducting vortex lattices. How many vortices are enclosed in a magnetic unit cell?

### § Kubo formula for Hall conductance

§  $H = H_0 + \Delta H$ , where  $\Delta H = - \int d\mathbf{r} \frac{1}{c} \vec{j} \cdot \vec{A}$

(here  $\vec{A}$  is related to the external electric field  $\vec{E}$  through  $\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t}$ )

$$\hat{\vec{j}}(\vec{r}) = -\frac{ie\hbar}{2m} (\psi^*(\mathbf{r}) \nabla \psi(\mathbf{r}) - \nabla \psi^* \psi).$$

In the interaction picture

$$\begin{aligned} |\psi(t)\rangle_I &= T \exp \left[ -\frac{i}{\hbar} \int_{t_0}^t \Delta H(t') dt' \right] |\psi(t_0)\rangle_I \approx \left( 1 - \frac{i}{\hbar} \int_{t_0}^t \Delta H(t') dt' \right) |\psi(t_0)\rangle \\ \hat{\vec{j}}(\vec{r}, t) &= e^{iH_0 t / \hbar} \hat{\vec{j}}(\vec{r}) e^{-iH_0 t} \end{aligned}$$

we set as  $t_0 \rightarrow -\infty$ ,  $|\psi(t_0)\rangle$  is the ground state of  $H_0$

$$\Rightarrow \langle \vec{j}(\vec{r}, t) \rangle = \langle 0(t) | \hat{\vec{j}}(\vec{r}, t) | 0(t) \rangle$$

$$= \langle 0 | \left[ 1 + \frac{i}{\hbar} \int_{-\infty}^t \Delta H(t') dt' \right] \hat{\vec{j}}(\vec{r}, t) \left[ 1 - \frac{i}{\hbar} \int_{-\infty}^t \Delta H(t') dt' \right] | 0 \rangle$$

$$= \langle 0 | \hat{\vec{j}}(\vec{r}, t) | 0 \rangle + \frac{i}{\hbar} \int_{-\infty}^t dt' \langle 0 | [\Delta H(t'), \hat{\vec{j}}(\vec{r}, t)] | 0 \rangle$$

$$\Rightarrow \langle \vec{j}(\vec{r}, t) \rangle = -\frac{i}{\hbar} \int_{-\infty}^t dt' \langle 0 | [\hat{\vec{j}}(\vec{r}, t), \Delta H(t')] | 0 \rangle$$

**HW:** More precisely, the electric current formula above doesn't include the diamagnetic part. The true current

$$\vec{j}(\vec{r}) = -\frac{ie\hbar}{2m} (\psi^*(\vec{r}) \nabla \psi(\vec{r}) - \nabla \psi^* \psi) - \frac{e^2}{mc} \psi^* \psi \vec{A}$$

$$\Rightarrow \boxed{\vec{j}(\vec{r}, t) = -\frac{i}{\hbar} \int_{-\infty}^t dt' \langle 0 | [\hat{j}(\vec{r}, t), \Delta H(t')] | 0 \rangle - \frac{e^2}{mc} n \vec{A}}$$

$$\rightarrow \vec{j}(\vec{r}, t) = \frac{i}{\hbar} \int d\vec{r}' \int_{-\infty}^t dt' \langle 0 | [\hat{j}(\vec{r}, t), \hat{j}(\vec{r}', t')] | 0 \rangle \cdot \frac{\vec{A}(\vec{r}', t')}{c} - \frac{ne^2}{mc} \vec{A}(\vec{r}, t)$$

$$\rightarrow = \sum_{q'} \frac{i}{\sqrt{\hbar c}} \int_{-\infty}^t dt' \langle 0 | [\hat{j}(\vec{r}, t), \hat{j}_\alpha(-q', t')] | 0 \rangle A_\alpha(q', t') - \frac{ne^2}{mc} \vec{A}(\vec{r}, t)$$

$$\Rightarrow j_\alpha(\vec{q}, t) = \frac{i}{\sqrt{\hbar c}} \int_{-\infty}^{+\infty} dt' \Theta(t-t') \underbrace{\langle 0 | [\hat{j}_\alpha(q, t), \hat{j}_\beta(-q, t')] | 0 \rangle}_{\text{only depend on } t-t'} A_\beta(q, t') + \frac{ne^2}{mc} A_\alpha(\vec{q}, t)$$

$$\text{Define } D_{\alpha\beta}(t-t') = \frac{i}{\sqrt{\hbar}} \Theta(t-t') \langle 0 | [\hat{j}_\alpha(q, t), \hat{j}_\beta(-q, t')] | 0 \rangle$$

$$\text{then } j_\alpha(\vec{q}, t) = \frac{1}{c} \int_{-\infty}^{+\infty} dt' D_{\alpha\beta}(t-t') A_\beta(\vec{q}, t') - \frac{ne^2}{mc} A_\alpha(\vec{q}, t)$$

Define Fourier transform

$$j_\alpha(\vec{q}, t) = \int \frac{dw}{2\pi} j_\alpha(\vec{q}, \omega) e^{-i\omega t}$$

$$D_{\alpha\beta}(t-t') = \int \frac{dw}{2\pi} D_{\alpha\beta}(q, w) e^{-i(wt-t')}$$

$$A_\beta(q, t') = \int \frac{dw'}{2\pi} A_\beta(q, w') e^{-iw't'}$$

$$\Rightarrow j_\alpha(\vec{q}, t) = \frac{1}{c} \int_{-\infty}^{+\infty} dt' \int \frac{dw, dw'}{(2\pi)^2} D_{\alpha\beta}(q, w) A_\beta(q, w') e^{-iwt} e^{i(w-w')t'}$$

$$- \frac{ne^2}{mc} A_\alpha(\vec{q}, t)$$

$$= \frac{1}{c} \int_{-\infty}^{+\infty} \frac{dw}{2\pi} D_{\alpha\beta}(q, w) A_\beta(q, w) e^{-iwt} - \frac{ne^2}{mc} \int_{-\infty}^{+\infty} \frac{dw}{2\pi} A_\alpha(\vec{q}, w) e^{-iwt}$$

$$\Rightarrow j_\alpha(\vec{q}, w) = [D_{\alpha\beta}(q, w) - \frac{ne^2}{m} \delta_{\alpha\beta}] \frac{1}{c} A_\beta(\vec{q}, w)$$

$$\text{According to } \vec{E} = -\frac{1}{c} \partial_t \vec{A} \Rightarrow \vec{E}(\vec{q}, w) = +\frac{iw}{c} \vec{A}(\vec{q}, w)$$

$$\Rightarrow j_\alpha(\vec{q}, w) = \frac{1}{i\omega} [D_{\alpha\beta}(q, w) - \frac{ne^2}{m} \delta_{\alpha\beta}] E_\beta(\vec{q}, w)$$

$$\text{or } \sigma_{\alpha\beta}(\vec{q}, w) = \frac{1}{i\omega} D_{\alpha\beta}(q, w) + \frac{ne^2}{mw} i \delta_{\alpha\beta}$$

$$= \frac{1}{i\omega V} \int_{-\infty}^{+\infty} dt' \left( \frac{+i}{\hbar} \right) \theta(t-t') \langle 0 | [\hat{j}_\alpha(\vec{q}, t), \hat{j}_\beta(-\vec{q}, t')] | 0 \rangle e^{i\omega(t-t')}$$

$$+ i \frac{ne^2}{mw} \delta_{\alpha\beta}$$

$$\sigma_{\alpha\beta}(\vec{q}, w) = \frac{1}{i\omega V} \int_{-\infty}^{+\infty} dt' \theta(t-t') e^{i(\omega+i\eta)(t-t')} \langle 0 | [\hat{j}_\alpha(\vec{q}, t), \hat{j}_\beta(-\vec{q}, t')] | 0 \rangle$$

$$+ \frac{ine^2}{mw} \delta_{\alpha\beta}$$

Now we use the Lehman representation

$$\begin{aligned}\sigma_{\alpha\beta}(\vec{q}, \omega) &= \frac{1}{\hbar\omega V} \int_0^{+\infty} dt e^{i(\omega+i\eta)t} \left\{ \langle 0 | j_\alpha(q) | n \rangle \langle n | j_\beta(-q) | 0 \rangle e^{-i(E_n - E_0)t} \right. \\ &\quad \left. - \langle 0 | j_\beta(-q) | n \rangle \langle n | j_\alpha(q) | 0 \rangle e^{i(E_n - E_0)t} \right\} \\ &+ \frac{i ne^2}{m\omega} \delta_{\alpha\beta} \\ &= \frac{1}{\hbar\omega V} \sum_n \frac{-\langle 0 | j_\alpha(q) | n \rangle \langle n | j_\beta(-q) | 0 \rangle}{i[\omega + i\eta - \frac{(E_n - E_0)}{\hbar}]} + \frac{\langle 0 | j_\beta(-q) | n \rangle \langle n | j_\alpha(q) | 0 \rangle}{i[\omega + i\eta + \frac{(E_n - E_0)}{\hbar}]}\end{aligned}$$

Set  $\vec{q} = 0$ ,

$$\begin{aligned}\sigma_{\alpha\beta}(\omega) &= \frac{i}{\omega V} \sum_n \left\{ \frac{\langle 0 | j_\alpha | n \rangle \langle n | j_\beta | 0 \rangle}{\hbar\omega + i\eta - (E_n - E_0)} - \frac{\langle 0 | j_\beta | n \rangle \langle n | j_\alpha | 0 \rangle}{\hbar\omega + i\eta + (E_n - E_0)} \right\} \\ &\quad + \frac{i ne^2}{m\omega} \delta_{\alpha\beta}\end{aligned}$$

For Hall conductance, set  $\omega \rightarrow 0$ ,  $\alpha = x$  and  $\beta = y$

$$\frac{1}{\hbar\omega - (E_n - E_0)} = \frac{-i}{E_n - E_0} - \frac{\hbar\omega}{(E_n - E_0)^2}$$

$$\frac{1}{\hbar\omega + (E_n - E_0)} = \frac{i}{E_n - E_0} - \frac{\hbar\omega}{(E_n - E_0)^2}$$

$$\Rightarrow \boxed{\sigma_{xy} = \frac{i\hbar}{V} \sum_{n \neq 0} \frac{\langle 0 | j_y | n \rangle \langle n | j_x | 0 \rangle - \langle 0 | j_x | n \rangle \langle n | j_y | 0 \rangle}{(E_n - E_0)^2}}$$

\* Consider  $H = \frac{(\vec{P} - \frac{e}{c}\vec{A})^2}{2m}$

$$\psi_{\alpha, \vec{k}}(\vec{r}) = e^{ik_x x + ik_y y} u_{\alpha, \vec{k}}(\vec{r}), \text{ with } H \psi_{\alpha, \vec{k}}(\vec{r}) = E_{\alpha}(\vec{k}) \psi_{\alpha, \vec{k}}(\vec{r})$$

$$\underbrace{\left[ e^{-i\vec{k} \cdot \vec{r}} H e^{i\vec{k} \cdot \vec{r}} \right]}_{\hat{H}(\vec{k})} u_{\alpha, \vec{k}}(\vec{r}) = E_{\alpha}(\vec{k}) \psi_{\alpha, \vec{k}}(\vec{r})$$

$$\Rightarrow \boxed{\hat{H}(\vec{k}) u_{\alpha, \vec{k}}(\vec{r}) = E_{\alpha}(\vec{k}) u_{\alpha, \vec{k}}(\vec{r})}$$

$\alpha$ -band index,  $\vec{k} = (k_x, k_y)$  labels states in a magnetic Brillouin zone.

$$\hat{\psi}(r) = \sum_{\vec{k}, \alpha} e^{i\vec{k} \cdot \vec{r}} u_{\alpha, \vec{k}}(\vec{r}) c_{\alpha}(\vec{k})$$

field operator

$$\Rightarrow \hat{j}(\vec{r}) = \frac{e}{2m} [\hat{\psi}^{\dagger}(r) [-i\hbar \nabla - \frac{e}{c} \vec{A}(r)] \hat{\psi}(r) - [-i\hbar \nabla + \frac{e}{c} \vec{A}(r)] \hat{\psi}^{\dagger}(r) \hat{\psi}(r)]$$

$$\hat{j}(q=0) = \int d^3 \vec{r} \hat{j}(\vec{r}) = \int d^3 \vec{r} \sum_{\vec{k}, \alpha} \sum_{\vec{k}' \beta'} \frac{e}{m} \left[ \overline{e^{i\vec{k} \cdot \vec{r}}} u_{\alpha, \vec{k}}^*(r) \left( -i\hbar \nabla - \frac{e}{c} \vec{A} \right) \right. \\ \left. e^{i\vec{k}' \cdot \vec{r}} u_{\beta, \vec{k}'}(r) \right] c_{\alpha, \vec{k}}^+ c_{\beta, \vec{k}'}$$

$$= \frac{e}{m} \sum_{\vec{k} \alpha, \vec{k}' \beta'} c_{\alpha, \vec{k}}^+ c_{\beta, \vec{k}'} \langle \vec{k} \alpha | \hat{v} | \vec{k}' \beta \rangle$$

$$\text{where } |\vec{k} \alpha\rangle = e^{i\vec{k} \cdot \vec{r}} u_{\alpha, \vec{k}}(\vec{r})$$

$$\text{and } \langle \vec{k} \alpha | \hat{v} | \vec{k}' \beta \rangle = \int d^3 r \left( u_{\alpha, \vec{k}}(\vec{r}) e^{i\vec{k} \cdot \vec{r}} \right)^* \left( -i\hbar \nabla - \frac{e}{mc} \vec{A} \right) \left( e^{i\vec{k}' \cdot \vec{r}} u_{\beta, \vec{k}'}(\vec{r}) \right)$$

Since magnetic translation  $\hat{T}_R$  commutes with  $\hat{v}$  - velocity operator,

$$[\hat{T}_R, \hat{v}] = 0 \Rightarrow \hat{T}_R (\hat{v} | k_\alpha \rangle) = \hat{v} \hat{T}_R | k_\alpha \rangle = e^{i \vec{k} \cdot \vec{R}} (\hat{v} | k_\alpha \rangle)$$

$$\Rightarrow \langle k_\alpha | \hat{v} | k_\beta \rangle = \delta_{kk'} \langle k_\alpha | \hat{v} | k_\beta \rangle$$

$$\begin{aligned} \text{where } \langle k_\alpha | \hat{v} | k_\beta \rangle &= \int d^3r \ u_{k_\alpha}^*(\vec{r}) \bar{e}^{ikr} \left[ -i\hbar \nabla - \frac{e}{mc} \vec{A} \right] (e^{ikr} u_{k_\beta}(\vec{r})) \\ &= \int d^3r \ u_{k_\alpha}^*(\vec{r}) \left[ -\frac{i\hbar \nabla}{m} + \frac{\hbar \vec{k}}{m} - \frac{e}{mc} \vec{A} \right] u_{k_\beta}(\vec{r}) \\ &= \int d^3r \ u_{k_\alpha}^*(\vec{r}) \frac{\partial H(\vec{k})}{\partial \vec{k}} u_{k_\beta}(\vec{r}) \quad \text{Exercise: prove it} \\ &= \boxed{\langle u_{k_\alpha} | \frac{\partial H(\vec{k})}{\partial \vec{k}} | u_{k_\beta} \rangle} = \langle k_\alpha | \hat{v} | k_\beta \rangle \end{aligned}$$

For non-interacting system:  $|n\rangle = c_{\alpha,k}^\dagger c_{\beta,k} |0\rangle \leftarrow$  since  $j(g=0)$  conserved  $\vec{k}$

$$\Rightarrow \sigma_{xy} = \frac{i\hbar e^2}{4V} \sum_{\substack{\alpha, \beta \\ E_\alpha(k) > E_F > E_\beta(k)}} \frac{\langle k_\alpha | v_y | k_\beta \rangle \langle k_\beta | v_x | k_\alpha \rangle - \langle k_\alpha | v_x | k_\beta \rangle \langle k_\beta | v_y | k_\alpha \rangle}{(E_\beta(k) - E_\alpha(k))^2}$$

$$E_\beta(k) > E_F > E_\alpha(k)$$

$$= \frac{i\hbar e^2}{Vh^2} \sum_{\substack{\alpha, \beta \\ E_\beta(k) > E_F > E_\alpha(k)}} \frac{\left\{ \langle u_{k_\alpha} | \frac{\partial H(k)}{\partial k_y} | u_{k_\beta} \rangle \langle u_{k_\beta} | \frac{\partial H(k)}{\partial k_x} | u_{k_\alpha} \rangle - \langle u_{k_\alpha} | \frac{\partial H(k)}{\partial k_x} | u_{k_\beta} \rangle \langle u_{k_\beta} | \frac{\partial H(k)}{\partial k_y} | u_{k_\alpha} \rangle \right\}}{(E_\beta(k) - E_\alpha(k))^2}$$

$$\text{Exercise : } \langle u_{k\alpha} | \frac{\partial H(k)}{\partial k_x} | u_{k\beta} \rangle = (E_k^\beta - E_k^\alpha) \langle u_{k\alpha} | \frac{\partial}{\partial k} u_{k\beta} \rangle$$

Prove

$$= -(E_k^\beta - E_k^\alpha) \langle \frac{\partial u_{k\alpha}}{\partial k} | u^\beta \rangle$$

$$\Rightarrow \sigma_{xy} = \frac{i e^2}{Vh} \sum_{E_\alpha(k) > E_F > E_\beta(k)} \left\{ \left\langle \frac{\partial u_{k\alpha}}{\partial k_y} | u_{k\beta} \rangle \langle u_{k\beta} | \frac{\partial u_{k\alpha}}{\partial k_x} \right\rangle \right. \\ \left. - \left\langle \frac{\partial u_{k\alpha}}{\partial k_x} | u_{k\beta} \rangle \langle u_{k\beta} | \frac{\partial u_{k\alpha}}{\partial k_y} \right\rangle \right\}$$

using  $\sum_{E_\alpha < E_F < E^\beta} |u_{k\alpha}\rangle \langle u_{k\alpha}| + |u_{k\beta}\rangle \langle u_{k\beta}| = 1 \leftarrow \text{for a fixed } k$

$$\Rightarrow \sigma_{xy} = \frac{i e^2}{Vh} \sum_{k, \alpha < E_F < \beta} \left\langle \frac{\partial u_{k\alpha}}{\partial k_y} \left| \frac{\partial u_{k\alpha}}{\partial k_x} \right. \right\rangle - \left\langle \frac{\partial u_{k\alpha}}{\partial k_x} \left| \frac{\partial u_{k\alpha}}{\partial k_y} \right. \right\rangle \\ - \underbrace{\left\langle \frac{\partial u_{k\alpha}}{\partial k_y} | u_{k\alpha} \rangle \langle u_{k\alpha} | \frac{\partial u_{k\alpha}}{\partial k_x} \right\rangle + \left\langle \frac{\partial u_{k\alpha}}{\partial k_x} | u_{k\alpha} \rangle \langle u_{k\alpha} | \frac{\partial u_{k\alpha}}{\partial k_y} \right\rangle}_{=0}$$

The 2nd line :  $\left\langle \frac{\partial u_{k\alpha}}{\partial k_y} | u_{k\alpha} \rangle = - \langle u_{k\alpha} | \frac{\partial u_{k\alpha}}{\partial k_y} \right\rangle \Rightarrow \text{the 2nd line} = 0$

$$\langle u_{k\alpha} | \frac{\partial u_{k\alpha}}{\partial k_x} \rangle = - \langle \frac{\partial u_{k\alpha}}{\partial k_x} | u_{k\alpha} \rangle$$

$$\Rightarrow \sigma_{x,y} = \frac{i e^2}{Vh} \sum_{\alpha < E_F} \sum_k \left\langle \frac{\partial u_{k\alpha}}{\partial k_y} \left| \frac{\partial u_{k\alpha}}{\partial k_x} \right. \right\rangle - \left\langle \frac{\partial u_{k\alpha}}{\partial k_x} \left| \frac{\partial u_{k\alpha}}{\partial k_y} \right. \right\rangle$$

$$= \frac{i e^2}{h} \sum_{\alpha < E_F} \int \frac{d^2 k}{(2\pi)^2} \left[ \partial_{k_x} \langle u_{k\alpha} | \partial_{k_y} u_{k\alpha} \rangle - \partial_{k_y} \langle u_{k\alpha} | \partial_{k_x} u_{k\beta} \rangle \right]$$

(10)

Define Berry connection

$$\vec{A}_\alpha(\vec{k}) = \langle u_{k,\alpha} | \vec{i}\partial_k | u_{k,\beta} \rangle$$

$$= \int d^2r \quad u_{k,\alpha}^* (\vec{i}\partial_k) u_{k,\beta}$$

$\Rightarrow$

$$\sigma_{xy} = \frac{e^2}{h} \cdot \frac{1}{2\pi} \sum_{\alpha < E_F} \int \left[ \partial_{k_x} A_{k_y}(\vec{k}) - \partial_{k_y} A_{k_x}(\vec{k}) \right] d^2k$$

$$\sigma_{xy} = \frac{e^2}{h} \sum_{\alpha < E_F} C_\alpha, \quad \text{with} \quad C_\alpha = \frac{1}{2\pi} \int d^2k \left( \nabla_{\vec{k}} \times \vec{A}(\vec{k}) \right)_z$$

\*  $C_\alpha$ : the Chern # associated with the  $\alpha$ -band!

\* Quantum mechanical WF can only be well-defined up to a phase. For a different phase convention

$$|u_{\vec{k}}\rangle \rightarrow |u'_{\vec{k}}\rangle = e^{i\Theta(\vec{k})} |u_{\vec{k}}\rangle$$

It's easy to show that  $\vec{A}'(\vec{k}) = \vec{A}(\vec{k}) + \partial_k \Theta(\vec{k})$ ,

thus  $\Omega_{xy}$  is invariant.

\* If  $|u_{\vec{k}}\rangle$  is regularly defined over the entire BZ, then

$\vec{A}(\vec{k})$  is also regular. Since BZ has no boundary, we have

$$C_\alpha = \frac{1}{2\pi} \int d^2k \left( \nabla_{\vec{k}} \times \vec{A}(\vec{k}) \right)_{\hat{z}} = 0.$$

\* In order to have non-zero  $C_\alpha$ ,  $|u_{\vec{k}}\rangle$  cannot be smoothly well-defined in the BZ. To understand it, let us use the spin-1/2 Berry phase example. The state  $\hat{n} \cdot \vec{\sigma} |\psi(\hat{n})\rangle = |\psi(\hat{n})\rangle \rightarrow$

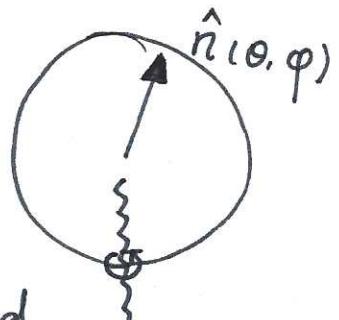
$$|\psi(\hat{n})\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

we define  $|\psi(\hat{n})\rangle$  in the following convention

that  $\langle \uparrow | \psi(\hat{n}) \rangle > 0$ . Nevertheless, there's a bad

point at  $\hat{n}$  on the south pole, where  $\cos \frac{\theta}{2} = 0$ . As a result, the phase

of  $|\psi(\hat{n})\rangle$  is not well-defined! Look at the  $\sigma_z$ -component —  $\dot{\phi}$  is not



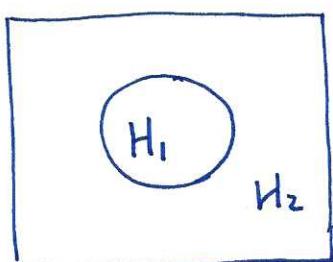
This corresponds to the gauge that a Dirac string located at the south pole. Around the Dirac string, phase varies  $2\pi$ .

\* For the case  $|U_k^{(\omega)}\rangle$ , we can choose a location  $\vec{r}_0$  inside the magnetic unit cell. The phase convention is that  $\langle \vec{r}_0 | U_k^{(\omega)} \rangle > 0$ .

Nevertheless, if there exist a point  $\vec{r}_0$ , such that  $\langle \vec{r}_0 | U_{k_0}^{(\omega)} \rangle = 0$ , then the phase of  $|U_{k_0}^{(\omega)}\rangle$  cannot be determined. Then  $\sigma_{xy}^{(\omega)}$  is given by the total vorticity of  $\langle \vec{r}_0 | U_k^{(\omega)} \rangle$  as a function of  $k$  lying the BZ.

As an example, consider the case that  $\langle \vec{r}_0 | U_k^{(\omega)} \rangle$  only vanishes at one point  $\vec{r}_0$  in the BZ. We divide the BZ

into two parts  $S_1$  and  $S_2$



① inside  $H_1$ ,  $\langle \vec{r}_1 | U_k^{(\omega)} \rangle > 0$ , the phase of  $|U_k^{(\omega)}\rangle$  is well-defined with respect to a point  $\vec{r}_1$

② inside  $H_2$ ,  $\langle \vec{r}_0 | U_k^{(\omega)} \rangle > 0$ ,  $|U_k^{(\omega)}\rangle$ 's phase well-defined respect to  $\vec{r}_0$ .

This corresponds to different choices of gauge. However, there's no a gauge the  $\vec{A}$  can be defined smoothly and uniquely.

At the boundary  $H_1$  and  $H_2$ , there's a phase mismatch

$|u_{\vec{k}}^{\text{II}}\rangle = e^{iX(\vec{k})} |u_{\vec{k}}^{\text{I}}\rangle$ , where  $X(\vec{k})$  is a smooth function on  $\partial H$ .

$$\text{on } \partial H, \quad \vec{A}_{\text{II}}(\vec{k}) = \vec{A}_{\text{I}}(\vec{k}) + \nabla_{\vec{k}} X(\vec{k})$$

$$\begin{aligned} \Rightarrow \sigma_{xy}^{(\omega)} &= \frac{e^2}{h} \frac{1}{2\pi} \left[ \int_{H_1} d^2k (\nabla_{\vec{k}} \times \vec{A}_{\text{I}})_3 + \int_{H_2} d^2k (\nabla_{\vec{k}} \times \vec{A}_{\text{II}})_3 \right] \\ &= \frac{e^2}{h} \frac{1}{2\pi} \oint_{\partial H} [A_{\text{I}}(\vec{k}) - A_{\text{II}}(\vec{k})] dk = \frac{e^2}{h} \frac{1}{2\pi} \oint \nabla_{\vec{k}} X \cdot d\vec{k} \\ &= \frac{e^2}{h} n \quad \text{where } n = \frac{1}{2\pi} \oint_{\partial H} d\vec{k} \cdot \nabla_{\vec{k}} X \leftarrow \text{the winding number} \end{aligned}$$