CH. 3 : TOPOLOGICAL BAND THEORY IN TWO DIMENSIONS

1) Quantized Hall conductivity of 2D insulators

Electric current density :

$$\vec{j} = \frac{e}{\underbrace{A}_{\text{area of sample}}} \sum_{\substack{\vec{k} \\ \in 1BZ}} \sum_{n} \langle \psi_{\vec{k}n} | \underbrace{\vec{v}}_{\text{velocity operator}} | \underbrace{\psi_{\vec{k}n}}_{\text{Bloch state}} \rangle \underbrace{f_{\vec{k}n}}_{e^- \text{ occupation factor}}$$

$$\vec{k} = (k_x, k_y)$$

* In equilibrium :

$$\langle \psi_{\vec{k}n} | \vec{v} | \psi_{\vec{k}n} \rangle = \frac{1}{\hbar} \frac{\partial E_{\vec{k}n}}{\partial \vec{k}}$$

$E_{\vec{k}n}$ = energy of an e^-

$$f_{\vec{k}n} = \frac{1}{e^{\beta(E_{\vec{k}n} - \mu)} + 1}$$

$$\vec{j} = 0 .$$

* Apply an electric field $\vec{E}$.

$$j_\alpha = \sum_\beta \underbrace{\sigma_{\alpha\beta}}_{\text{conductivity}} E_\beta$$

$\alpha, \beta \in \{x, y\}$

We want to calculate $\sigma_{\alpha\beta}$ using perturbation theory.

Hamiltonian:

$$\mathcal{H} = \underbrace{\mathcal{H}_0}_{\substack{\text{crystal} \\ \text{in equilibrium}}} + \underbrace{\delta\mathcal{H}}_{\text{effect of } \vec{E}}$$

Consider $\vec{E} = E\,\hat{x}$

(dc, uniform)

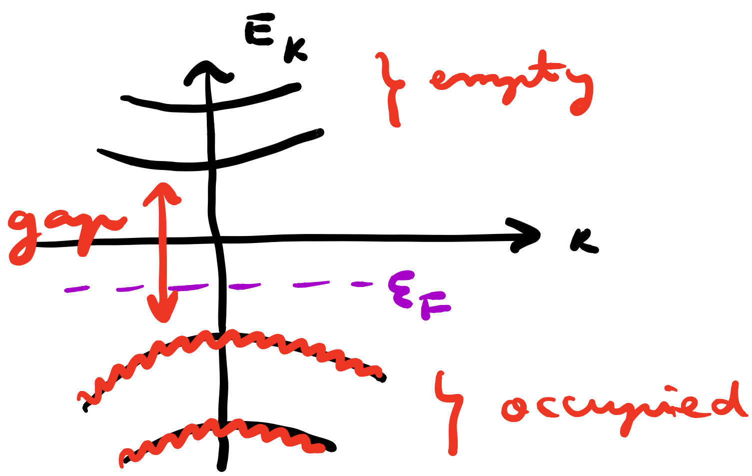
$$\Rightarrow \quad \delta\mathcal{H} = e\,E\,\underbrace{x}_{\substack{\text{position operator} \\ \text{(x-component)}}}$$

$\delta \mathcal{H}$ changes eigenstates and eigenvalues.

$$\vec{j} = \frac{e}{A} \sum_{\vec{k}n} \delta \left(\langle \psi_{\vec{k}n} | \vec{v} | \psi_{\vec{k}n} \rangle \right) f_{\vec{k}n}$$

$$+ \frac{e}{A} \sum_{\vec{k}n} \langle \psi_{\vec{k}n} | \vec{v} | \psi_{\vec{k}n} \rangle \, \delta f_{\vec{k}n}$$

Insulator in equilibrium at $T=0$:



A weak, dc electric field cannot change the occupancy

$$\Rightarrow \quad \delta f_{\vec{k}n} = 0$$

$$\Rightarrow \quad \vec{J} = \frac{e}{A} \sum_{\vec{k}n} \delta \left(\langle \psi_{\vec{k}n} | \vec{v} | \psi_{\vec{k}n} \rangle \right) \underbrace{f_{\vec{k}n}}$$

Fermi - Dirac

$$* \quad \delta \left(\langle \psi_{\vec{k}n} | \vec{v} | \psi_{\vec{k}n} \rangle \right)$$

$$= \left(\delta \langle \psi_{\vec{k}n} | \right) \vec{v} \, | \psi_{\vec{k}n} \rangle$$

$$+ \cancel{\langle \psi_{\vec{k}n} | (\delta \vec{v}) | \psi_{\vec{k}n} \rangle} \rightarrow 0$$

$$+ \langle \psi_{\vec{k}n} | \vec{v} \, \delta | \psi_{\vec{k}n} \rangle$$

Note: $\delta \vec{v} = 0$

Proof:

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

$$= -\frac{i}{\hbar}[\vec{r}, \mathcal{H}_0 + \delta \mathcal{H}]$$

$[\vec{r}, x] = 0$

$$= -\frac{i}{\hbar}[\vec{r}, \mathcal{H}_0]$$

= unperturbed velocity operator.

* $\delta |\psi_{\vec{k}n}\rangle =$

$$= \sum_{n' \neq n} |\psi_{\vec{k}n'}\rangle \frac{\langle \psi_{\vec{k}n'} | eEx | \psi_{\vec{k}n}\rangle}{E_{\vec{k}n} - E_{\vec{k}n'}}$$

(i) At first glance it is not obvious why $\delta\mathcal{H}$ does not couple eigenstates of different crystal momentum.

(ii) We assume all bands to be non degenerate. This assumption can be relaxed and the final result does not change.

Plug this in the expression for $\vec{j}$:

$$* \quad j_\alpha = \frac{e^2 E}{A} \sum_{\substack{m,m' \\ (m \neq m')}} \sum_{\vec{k}}$$

$$\left[\frac{\langle \psi_{\vec{k}m'} | v_\alpha | \psi_{\vec{k}m} \rangle \langle \psi_{\vec{k}m} | x | \psi_{\vec{k}m'} \rangle f_{\vec{k}m}}{E_{\vec{k}m} - E_{\vec{k}m'}} \right.$$

$$\left. + \frac{\langle \psi_{\vec{k}m} | v_\alpha | \psi_{\vec{k}m'} \rangle \langle \psi_{\vec{k}m'} | x | \psi_{\vec{k}m} \rangle f_{\vec{k}m}}{E_{\vec{k}m} - E_{\vec{k}m'}} \right]$$

$=$

$\uparrow$

interchange

$m \leftrightarrow m'$ in

the 2nd term

$$= \frac{e^2 E}{A} \sum_{n,n'} \sum_{\vec{k}}$$

$$\frac{\langle \psi_{\vec{k}n'} | v_\alpha | \psi_{\vec{k}n} \rangle \langle \psi_{\vec{k}n} | x | \psi_{\vec{k}n'} \rangle}{E_{\vec{k}n} - E_{\vec{k}n'}}$$

$$\left(f_{\vec{k}n} - f_{\vec{k}n'} \right)$$

$$= j_\alpha$$

* Rewrite matrix element of position operator:

$$\langle \psi_{\vec{k}n} | v_x | \psi_{\vec{k}n'} \rangle =$$

$$= - \frac{i}{\hbar} \langle \psi_{\vec{k}n} | [x, \mathcal{H}_0] | \psi_{\vec{k}n'} \rangle$$

$$= -\frac{i}{\hbar}\left(E_{\vec{k}m'} - E_{\vec{k}m}\right)\langle \psi_{\vec{k}m} | \underbrace{x}_{\text{position.}} | \psi_{\vec{k}m'} \rangle$$

$$[A, B] = AB - BA$$

$$\mathcal{H}_0 | \psi_{\vec{k}m} \rangle = E_{\vec{k}m} | \psi_{\vec{k}m} \rangle$$

$$\Rightarrow \langle \psi_{\vec{k}m} | x | \psi_{\vec{k}m'} \rangle =$$

$$= i\hbar \, \frac{\langle \psi_{\vec{k}m} | v_x | \psi_{\vec{k}m'} \rangle}{E_{\vec{k}m} - E_{\vec{k}m'}}$$

$$(\text{for } E_{\vec{k}m} \neq E_{\vec{k}m'})$$

* Then,

$$j_\alpha = -\frac{i e^2 \hbar E}{A} \sum_{n,n'} \sum_{\vec{k}}$$

$$(f_{\vec{k}n} - f_{\vec{k}n'}) \frac{\langle \psi_{\vec{k}n} | v_x | \psi_{\vec{k}n'} \rangle \langle \psi_{\vec{k}n'} | v_\alpha | \psi_{\vec{k}n} \rangle}{(E_{\vec{k}n} - E_{\vec{k}n'})^2}$$

$$* \quad \sigma_{\alpha x} =$$

$$= -\frac{i e^2 \hbar}{A} \sum_{\substack{n,n' \\ (n \neq n')}} \sum_{\vec{k}} (f_{\vec{k}n} - f_{\vec{k}n'})$$

$$\frac{\langle \psi_{\vec{k}n} | v_x | \psi_{\vec{k}n'} \rangle \langle \psi_{\vec{k}n'} | v_\alpha | \psi_{\vec{k}n} \rangle}{(E_{\vec{k}n} - E_{\vec{k}n'})^2}$$

$$= -\frac{ie^2\hbar}{A}\sum_{n,n'}\sum_{\vec{k}}\frac{f_{\vec{k}n}}{(E_{\vec{k}n}-E_{\vec{k}n'})^2}$$

$$\left[\langle\psi_{\vec{k}n}|v_x|\psi_{\vec{k}n'}\rangle\langle\psi_{\vec{k}n'}|v_\alpha|\psi_{\vec{k}n}\rangle - (n\leftrightarrow n')\right]$$

$$= \frac{2e^2\hbar}{A}\sum_{n,n'}\sum_{\vec{k}}\frac{f_{\vec{k}n}}{(E_{\vec{k}n}-E_{\vec{k}n'})^2}$$

$$\mathrm{Im}\left[\langle\psi_{\vec{k}n}|v_x|\psi_{\vec{k}n'}\rangle\langle\psi_{\vec{k}n'}|v_\alpha|\psi_{\vec{k}n}\rangle\right]$$

$$\underset{T\to 0}{=}$$

$$= \frac{2e^2\hbar}{A} \sum_{n \in occ} \sum_{n' \neq n}$$

$$\frac{\mathrm{Im}\left[\langle \psi_{\vec{k}n} | v_x | \psi_{\vec{k}n'} \rangle \langle \psi_{\vec{k}n'} | v_\alpha | \psi_{\vec{k}n} \rangle\right]}{\left(E_{\vec{k}n} - E_{\vec{k}n'}\right)^2}$$

$$= \sigma_{\alpha x}$$

$$\Rightarrow \boxed{\sigma_{xx} = 0}$$

Likewise, $\boxed{\sigma_{yy} = 0}$

The dc longitudinal conductivity of an insulator is zero at $T = 0$.

How about the Hall conductivity?

$$\sigma_{xy} = \frac{2e^2\hbar}{A} \sum_{\vec{k}} \sum_{n \in occ} \sum_{n' \neq n} \frac{\mathrm{Im}\left[\langle \psi_{\vec{k}n} | v_x | \psi_{\vec{k}n'} \rangle \langle \psi_{\vec{k}n'} | v_y | \psi_{\vec{k}n} \rangle\right]}{\left(E_{\vec{k}n} - E_{\vec{k}n'}\right)^2}$$

* Write velocity matrix element as follows:

$$|\psi_{\vec{k}n}\rangle = e^{i\vec{k}\cdot\vec{r}} |u_{\vec{k}n}\rangle$$

$$\langle \psi_{\vec{k}n} | \vec{v} | \psi_{\vec{k}n'} \rangle =$$

operator　　number

$$= \langle u_{\vec{k}n} | e^{-i\vec{k}\cdot\vec{r}}\, \vec{v}\, e^{i\vec{k}\cdot\vec{r}} | u_{\vec{k}n'} \rangle$$

$$e^{-i\vec{k}\cdot\vec{r}}\ \vec{v}\ e^{i\vec{k}\cdot\vec{r}} =$$

$$= -\frac{i}{\hbar}\, e^{-i\vec{k}\cdot\vec{r}} \left[\vec{r}, \mathcal{H}_0\right] e^{i\vec{k}\cdot\vec{r}}$$

$$= -\frac{i}{\hbar} \left[\vec{r}, \underbrace{e^{-i\vec{k}\cdot\vec{r}}\ \mathcal{H}_0\ e^{i\vec{k}\cdot\vec{r}}}_{\mathcal{H}_0(\vec{k})}\right]$$

$$= -\frac{i}{\hbar} \left[\vec{r}, \mathcal{H}_0(\vec{k})\right]$$

momentum operator

$$= -\frac{i}{\hbar} \Big[\vec{r}, \frac{(\vec{p} + \hbar\vec{k})^2}{2m} + V(\vec{r}) + \lambda_{so}\,(\vec{p} + \hbar\vec{k})\cdot(\vec{\sigma}\times\vec{\nabla}V)\Big]$$

$=$

$[\vec{r}, f(\vec{p})] = i\hbar \frac{\partial f}{\partial \vec{p}}$

$$= \frac{\vec{p} + \hbar\vec{k}}{m} + \lambda_{so}\, \vec{\sigma} \times \vec{\nabla} V$$

$$= \frac{1}{\hbar} \frac{\partial \varepsilon_0(\vec{k})}{\partial \vec{k}}$$

$$= e^{-i\vec{k}\cdot\vec{r}}\, \vec{v}\, e^{i\vec{k}\cdot\vec{r}} \equiv \vec{v}_{\vec{k}}$$

* Then,

$$\sigma_{xy} = \frac{2e^2}{A\hbar} \sum_{\vec{k}} \sum_{n \in occ} \sum_{n'} \frac{1}{\left(E_{\vec{k}n} - E_{\vec{k}n'}\right)^2}$$

$$\mathrm{Im}\left[\langle u_{\vec{k}n} | \frac{\partial \mathcal{H}_0}{\partial k_x} | u_{\vec{k}n'} \rangle \langle u_{\vec{k}n'} | \frac{\partial \mathcal{H}_0}{\partial k_y} | u_{\vec{k}n} \rangle \right]$$

$\Rightarrow$

$$\mathrm{Im}\, z = \frac{z - z^*}{2i}$$

$$\sigma_{xy} = \frac{-e^2}{A\hbar} \sum_{\vec{k}} \sum_{n \in occ} \hat{z} \cdot \underbrace{\vec{B}_n(\vec{k})}_{\text{Berry curvature for band } n \text{ at momentum } \vec{k}}$$

where

$$\vec{B}_n(\vec{k}) = i \sum_{\substack{n' \\ (n' \neq n)}}$$

cross product

$$\frac{\langle u_{\vec{k}n} | \frac{\partial \mathcal{H}_0}{\partial \vec{k}} | u_{\vec{k}n'} \rangle \times \langle u_{\vec{k}n'} | \frac{\partial \mathcal{H}_0}{\partial \vec{k}} | u_{\vec{k}n} \rangle}{(E_{\vec{k}n} - E_{\vec{k}n'})^2}$$

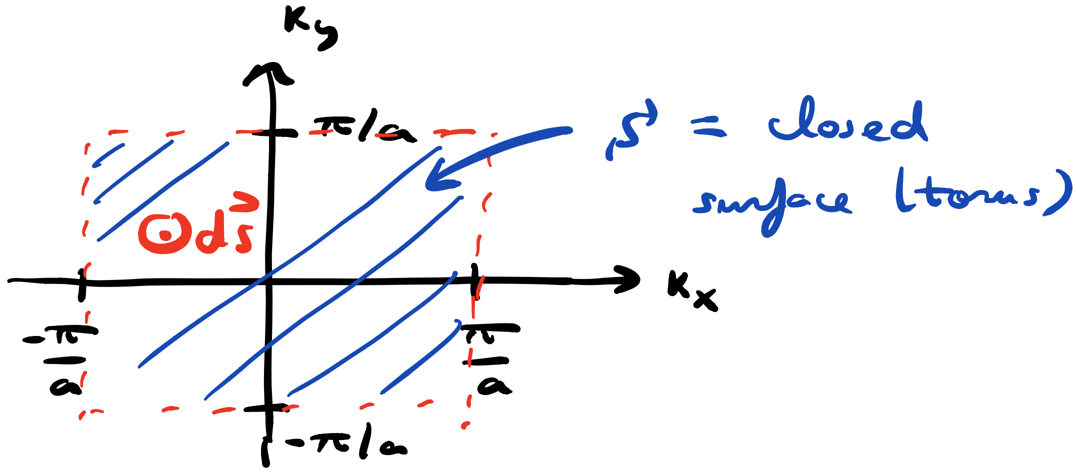
Using $\quad \frac{1}{A} \sum_{\vec{k}} \longrightarrow \int \frac{d^2k}{(2\pi)^2},$

$$\sigma_{xy} = -\frac{e^2}{\hbar} \sum_{n \in occ} \int \frac{d^2k}{(2\pi)^2} \hat{z} \cdot \vec{B}_n(\vec{k})$$

$$= -\frac{e^2}{\hbar} \sum_{n \in occ} \frac{1}{(2\pi)^2} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk_x \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk_y$$

suppose square lattice

$$\hat{z} \cdot \vec{B}_n(\vec{k})$$



$$\boxed{\sigma_{xy}} = -\frac{e^2}{\hbar} \sum_{n \in occ} \frac{1}{(2\pi)^2} \oint_S d\vec{S} \cdot \vec{B}_n(\vec{k})$$

$$= -\frac{e^2}{\hbar} \sum_{n \in occ} \frac{1}{2\pi} \underbrace{C_n}_{\text{Chern \# for band } n \text{ (integer)}}$$

$$= \boxed{\frac{e^2}{h} \times \text{integer}}$$

→ a fundamental constant!

$$\boxed{\text{integer} = - \sum_{n \in occ} C_n}$$

"TKNN formula"

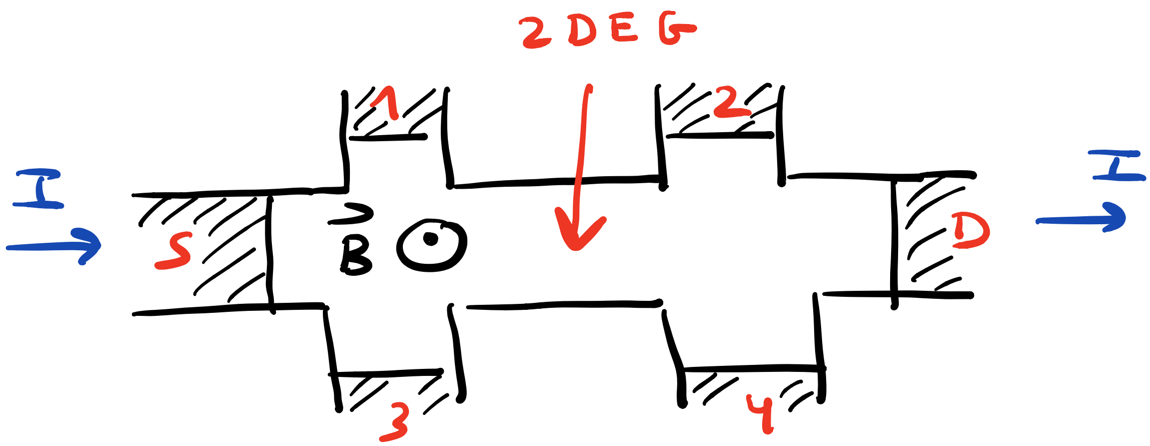
Thouless, Kohmoto, Nightingale, den Nijs, PRL 49, 405 (1982)

$$\vec{B}_n(\vec{k}) = -\vec{B}_n(-\vec{k})$$

if time-reversal symmetry is present

$\Rightarrow$ $C_n = 0$ in a crystal with time-reversal symmetry.

② Quantum Hall insulator

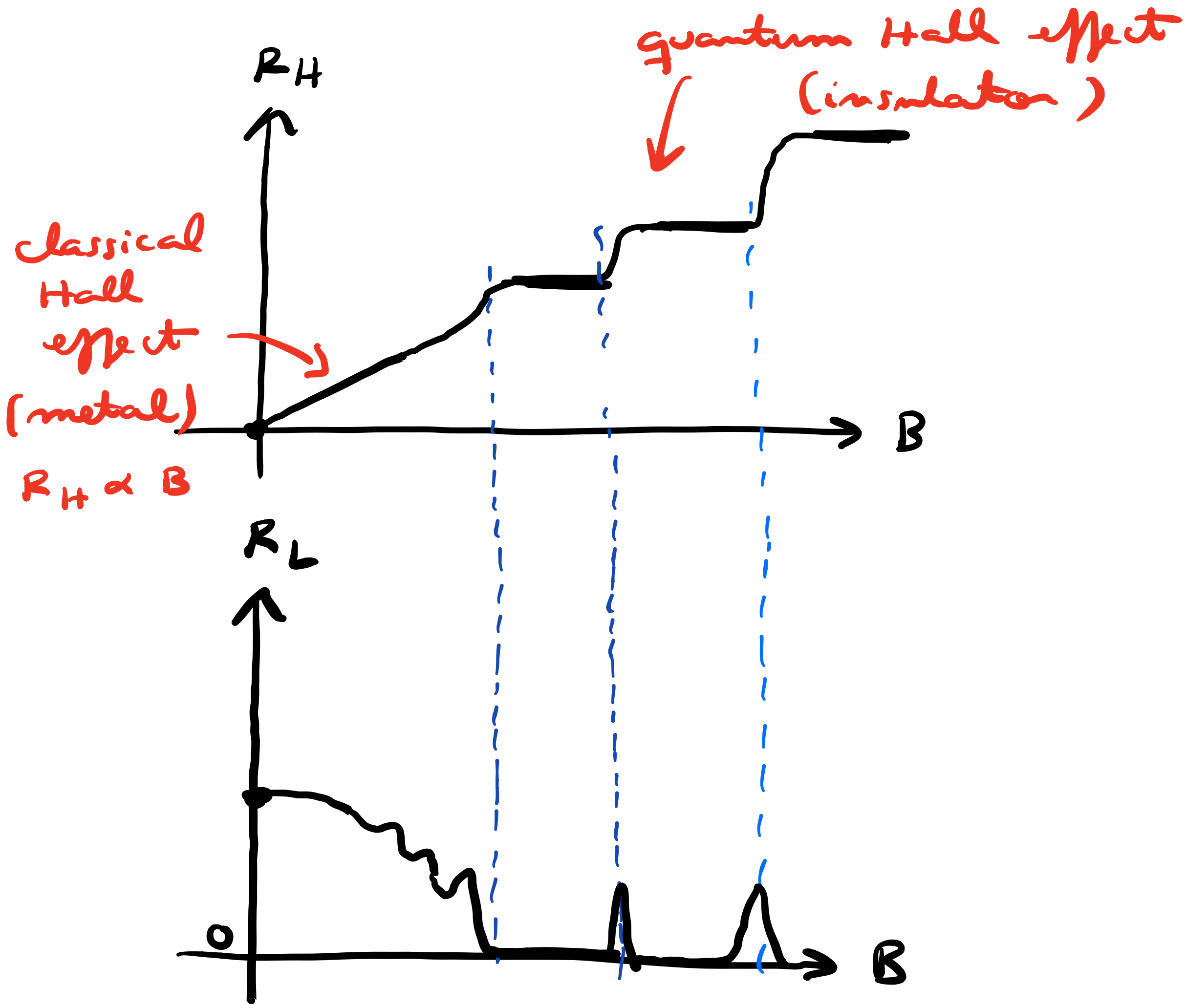


Longitudinal resistance:

$$R_L = \frac{V_2 - V_1}{I}$$

Hall resistance:

$$R_H = \frac{V_1 - V_3}{I}$$



Quantum Hall regime:

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

where $\nu = 1, 2, 3, \ldots$

$R_L = 0$ when R_H is in a plateau.

These findings are consistent w/ TKNN formula:

Resistivity tensor:

$$\overleftrightarrow{\rho} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix}$$

$$= \overleftrightarrow{\sigma}^{-1}$$

where

$\overleftrightarrow{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix}$ is

the conductivity tensor.

$$\Rightarrow \rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}^2}$$

$$\rho_{xy} = - \frac{\sigma_{xy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}^2}$$

For an insulator w/

$$\begin{cases} \sigma_{xx} = \sigma_{yy} = 0 \\ \sigma_{xy} \neq 0 \end{cases}$$

it follows that

$$\rho_{xx} = 0$$

$$\rho_{xy} = \frac{1}{\sigma_{xy}} = \frac{1}{\frac{e^2}{h} \times \text{integer}}$$

$$= \frac{h}{e^2 \times \text{integer}}$$