1.1.4. Quantization of the Hall conductivity

The Kubo formula

1. ∃ Unperturbed Hamiltonian H_0 with Eigenstates $|n\rangle$ and Eigenenergies E_n

   ∃ Time-dependent perturbation $\Delta H(t)$

   $\rightarrow \quad H = H_0 + \Delta H(t)$

2. Interaction picture:

$$\Delta H_I(t) = U_0^\dagger(t)\,\Delta H(t)\,U_0(t) \quad \text{and} \quad |\Psi(t)\rangle_I = U(t,t_0)\,|\Psi(t_0)\rangle_I$$

with $U_0(t) = e^{-\frac{i}{\hbar} H_0 t}$

and

$$U(t,t_0) = \mathcal{T}\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} \Delta H_I(t')\,dt'\right\}$$

3. Prepare system for $t_0 \to -\infty$ in ground state $|0\rangle$ of H_0

4. ✗ Expectation value of arbitrary operator $O_I(t) = U_0^\dagger O U_0$:

$$\langle O(t)\rangle = \langle 0| U^\dagger(t,-\infty)\, O_I(t)\, U(t,-\infty)|0\rangle$$

$$\approx \langle 0| \left\{ O_I(t) + \frac{i}{\hbar}\int_{-\infty}^{t} [\Delta H_I(t'), O_I(t)]\, dt' \right\} |0\rangle$$

→ Kubo formula:

$$\delta\langle O(t)\rangle := \langle O(t)\rangle - \langle O\rangle = \frac{i}{\hbar}\int_{-\infty}^{t} \langle 0|[\Delta H_I(t'), O_I(t)]|0\rangle\, dt'$$

5. ✗ Coupling to electric field $\vec{E}(t) = \vec{E}\cdot e^{-i\omega t}$

Choose gauge such that $\vec{E}(t) = -\partial_t \vec{A}(t)$ ⟵ ($\phi = \text{const}$)

→ $\vec{A}(t) = \vec{E}\, e^{-i\omega t}/(i\omega)$:

$$\Delta H_I(t) = -\vec{J}(t)\cdot\vec{A}(t)$$

with current operator $\vec{J}(t)$ ← (I-picture)

$$\frac{(\vec{p}+e\vec{A})^2}{2m} \approx \frac{p^2}{2m} + e\frac{\vec{p}\cdot\vec{A}}{m} + A^2, \qquad \frac{e\vec{p}}{m} \simeq \vec{J}$$

6. Current as observable: $O = J_i \longrightarrow$

$$\langle J_i(t)\rangle = -\frac{1}{\hbar\omega}\int_{-\infty}^{t}\langle 0|[J_j(t'), J_i(t)]|0\rangle E_j e^{-i\omega t'}dt'$$

$t'' = t - t'$, H_0 time-translation invariant

$$= \underbrace{\left\{\frac{1}{-\hbar\omega}\int_0^\infty \langle 0|[J_j(0), J_i(t'')]|0\rangle e^{i\omega t''}dt''\right\}}_{=\,\sigma_{ij}(\omega)}\cdot E_j e^{-i\omega t}$$

$= \sigma_{ij}(\omega)$ conductivity tensor

7. Hall conductivity:

$$\sigma_{xy}(\omega) = -\frac{1}{\hbar\omega}\int_0^\infty \langle 0|[J_y(0), J_x(t)]|0\rangle e^{i\omega t}dt$$

8. Use $U_0(t) = \sum_n e^{-iE_n t/\hbar} |n\rangle\langle n|$ and $J_i(t) = U_0^\dagger(t) J_i U_0(t)$:

$$\sigma_{xy}(\omega) = -\frac{1}{\hbar\omega} \int_0^\infty \sum_n \Big\{ \langle 0| J_y |n\rangle\langle n| J_x |0\rangle e^{i(E_n - E_0)t/\hbar} - \langle 0| J_x |n\rangle\langle n| J_y |0\rangle e^{i(E_0 - E_n)t/\hbar} \Big\} e^{i\omega t} dt$$

Regularize: $\omega \to \omega + i\varepsilon$

$$= \frac{i}{\omega} \sum_{n \neq 0} \left\{ \frac{\langle 0| J_y |n\rangle\langle n| J_x |0\rangle}{\hbar\omega + E_n - E_0} - \frac{\langle 0| J_x |n\rangle\langle n| J_y |0\rangle}{\hbar\omega + E_0 - E_n} \right\}$$

9. Take DC limit $\omega \to 0$ and use $\frac{1}{\hbar\omega - E_n - E_0} = \frac{1}{E_n - E_0} - \frac{\hbar\omega}{(E_n - E_0)^2} + O(\omega^2)$:

$$\sigma_{xy} \doteq -i\hbar \sum_{n \neq 0} \frac{\langle 0| J_y |n\rangle\langle n| J_x |0\rangle - \langle 0| J_x |n\rangle\langle n| J_y |0\rangle}{(E_n - E_0)^2}$$

Note:

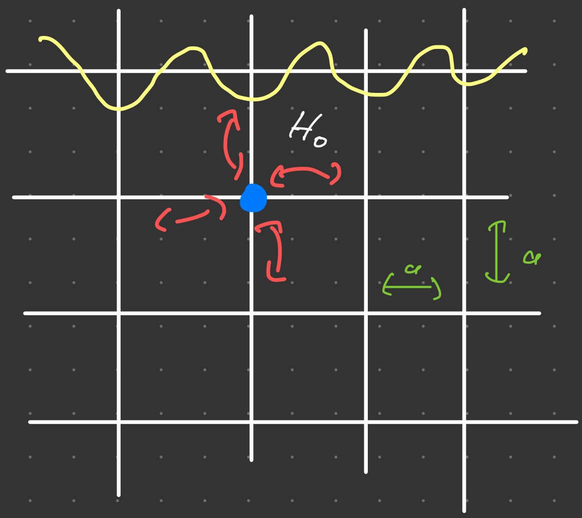
$$\sum_{n\neq 0} \frac{\langle 0|J_y|n\rangle\langle n|J_x|0\rangle + \langle 0|J_x|n\rangle\langle n|J_y|0\rangle}{E_n - E_0} = -\left(-\text{''}- \right) = 0$$

Rotation by $\frac{\pi}{2}$: $J_x \mapsto J_y$, $J_y \mapsto -J_x$

Rotation symmetry: $\sigma = R\sigma R^T \longrightarrow \sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix}$

The TKNN invariant

1. $\nexists$ Single electron in a periodic potential with Hamiltonian H_0:



2. Block theorem:

* Eigenfunctions $\psi_{n\vec{k}} = e^{i\vec{k}\vec{x}} u_{n\vec{k}}(x)$

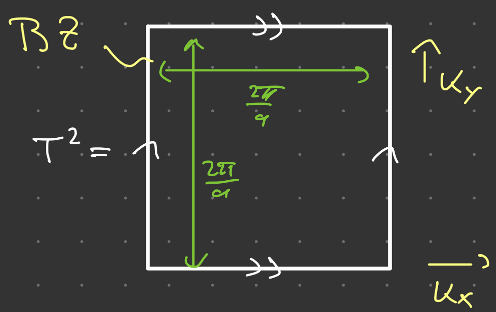
with $u_{n\vec{k}}(\vec{x}+\vec{R}) = u_{n\vec{k}}(\vec{x})$ for lattice vectors $\vec{R}$ and $n = 1, 2, 3, \ldots$ band index

* Eigenenergies $\varepsilon_n(\vec{k})$ continuous in $\vec{k} \rightarrow$ "Bands"

* $\psi_{n\,\vec{k}+\vec{K}} = \psi_{n\vec{k}}$

for reciprocal lattice vectors $\vec{K}$

$\rightarrow$ Brillouin zone = Torus T^2



3. Many-body Fock states with Fermi energy E_F:

Ground state $|0\rangle \mapsto |\underline{0}\rangle$ = Filled Fermi se

Excited states $|n\rangle \mapsto |\underline{n}\rangle$ = Fermi sea with particle-hole excitations

Current operator $J_i \mapsto \mathcal{J}_i$ = Second-quantized current operator

$\rightarrow$

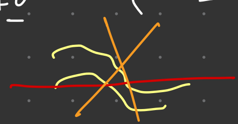
$$\sigma_{xy} = -i\hbar \sum_{\underline{n} \neq \underline{0}} \frac{\langle \underline{0} | \mathcal{J}_y | \underline{n} \rangle \langle \underline{n} | \mathcal{J}_x | \underline{0} \rangle - \langle \underline{0} | \mathcal{J}_x | \underline{n} \rangle \langle \underline{n} | \mathcal{J}_y | \underline{0} \rangle}{(E_{\underline{n}} - E_{\underline{0}})^2}$$

4. Current operator = Single-particle operator:

$$\mathcal{J}_i = \sum_{n\vec{k},\, m\vec{q}} \langle \psi_{n\vec{k}} | J_i | \psi_{m\vec{q}} \rangle \, c^\dagger_{n\vec{k}} c_{m\vec{q}}$$

$\rightarrow$

$$\sum_{\underline{n} \neq \underline{0}} \frac{\langle \underline{0} | \mathcal{J}_y | \underline{n} \rangle \langle \underline{n} | \mathcal{J}_x | \underline{0} \rangle}{(E_{\underline{n}} - E_{\underline{0}})^2} \hat{=} \sum_{n\vec{k},\, m\vec{q}} \frac{\langle \psi_{n\vec{k}} | J_x | \psi_{m\vec{q}} \rangle \langle \psi_{m\vec{q}} | J_x | \psi_{n\vec{k}} \rangle}{(\varepsilon_m(\vec{q}) - \varepsilon_n(\vec{k}))^2}$$



$\varepsilon_n(\vec{k}) < E_F < \varepsilon_m(\vec{q})$

$$\rightarrow \quad \sigma_{xy} = -i\hbar \sum_{\substack{n,m \\ \varepsilon_n < E_F < \varepsilon_m}} \int_{T^2} \frac{d^2k\, d^2q}{(2\pi)^4} \frac{\langle \psi_{n\vec{k}} | J_y | \psi_{m\vec{q}} \rangle \langle \psi_{m\vec{q}} | J_x | \psi_{n\vec{k}} \rangle - (x \leftrightarrow y)}{(\varepsilon_m(\vec{q}) - \varepsilon_n(\vec{k}))^2}$$

5. a) Define single-particle current operator:

$$\vec{J} := e\dot{\vec{x}} = i\frac{e}{\hbar}[H_0, \vec{x}]$$

b) ∃ Translation operator $T_{\vec{R}}$ / : (lattice vector)

$$T_R \vec{x} T_R^{-1} = \vec{x} + \vec{R}, \qquad T_R H_0 T_R^{-1} = H_0$$

and $T_R |\psi_{n\vec{k}}\rangle = e^{i\vec{k}\vec{R}} |\psi_{n\vec{k}}\rangle$

c) $T_{\vec{R}} \vec{J} T_{\vec{R}}^{-1} = i\frac{e}{\hbar}[H_0, \vec{x} + \vec{R}] = i\frac{e}{\hbar}[H_0, \vec{x}] = \vec{J}$

d) Thus

$$\sigma_{xy} = -i\hbar \sum_{\substack{n,m \\ \varepsilon_n < E_F < \varepsilon_m}} \int_{T^2} \frac{d^2k}{(2\pi)^2} \frac{\langle \psi_{n\vec{k}} | J_y | \psi_{m\vec{k}} \rangle \langle \psi_{m\vec{k}} | J_x | \psi_{n\vec{k}} \rangle - (x \leftrightarrow y)}{(\varepsilon_m(\vec{k}) - \varepsilon_n(\vec{k}))^2}$$

Bloch theorem

6. a) Use $|\psi_{n\vec{k}}\rangle = e^{i\vec{k}\vec{x}} |u_{n\vec{k}}\rangle$ and define $\tilde{J}(\vec{k}) := e^{-i\vec{k}\vec{x}} J e^{i\vec{k}\vec{x}}$

so that

$$\langle \psi_{n\vec{k}} | J_i | \psi_{m\vec{k}} \rangle = \langle u_{nk} | \tilde{J}_i(\vec{k}) | u_{m\vec{k}} \rangle$$

b) Define $\tilde{H}_0(\vec{k}) := e^{-i\vec{k}\vec{x}} H_0 e^{i\vec{k}\vec{x}}$ so that

$$H_0 |\psi_{n\vec{k}}\rangle = \varepsilon_n(\vec{k}) |\psi_{n\vec{k}}\rangle \Leftrightarrow \tilde{H}_0(\vec{k}) |u_{n\vec{k}}\rangle = \varepsilon_n(\vec{k}) |u_{n\vec{k}}\rangle$$

c) Then $\tilde{J}_i \stackrel{\circ}{=} \frac{e}{\hbar} \tilde{\partial}_i \tilde{H}_0$ where $\tilde{\partial}_i = \frac{\partial}{\partial k_i}$

d) Thus

$$\sigma_{xy} = -i\hbar \sum_{\substack{n,m \\ \varepsilon_n < E_F < \varepsilon_m}} \int_{T^2} \frac{d^2k}{(2\pi)^4} \frac{\langle u_{n\vec{k}} | \tilde{\partial}_y \hat{H}_0 | u_{m\vec{k}} \rangle \langle u_{m\vec{k}} | \tilde{\partial}_x \hat{H}_0 | u_{n\vec{k}} \rangle - (y \leftrightarrow x)}{(\varepsilon_m(\vec{k}) - \varepsilon_n(\vec{k}))^2}$$

7. Use

$$\langle u_{n\vec{k}} | \tilde{\partial}_y \hat{H}_0 | u_{m\vec{k}} \rangle = \langle u_{n\vec{k}} | \tilde{\partial}_y (\hat{H}_0 | u_{m\vec{k}} \rangle) - \langle u_{n\vec{k}} | \hat{H}_0 | \tilde{\partial}_y u_{m\vec{k}} \rangle$$

$$= [\varepsilon_m(\vec{k}) - \varepsilon_n(\vec{k})] \langle u_{n\vec{k}} | \tilde{\partial}_y u_{m\vec{k}} \rangle$$

$$= [\varepsilon_n(\vec{k}) - \varepsilon_m(\vec{k})] \langle \tilde{\partial}_y u_{n\vec{k}} | u_{m\vec{k}} \rangle$$

$$\longrightarrow \sigma_{xy} = -i\hbar \sum_{\substack{n,m \\ \varepsilon_n < E_F < \varepsilon_m}} \int_{T^2} \frac{d^2k}{(2\pi)^4} \left\{ \langle \tilde{\partial}_y u_{n\vec{k}} | u_{m\vec{k}} \rangle \langle u_{m\vec{k}} | \partial_x u_{n\vec{k}} \rangle - (x \leftrightarrow y) \right\}$$

8. $\sum_m |u_{m\vec{k}} \times u_{m\vec{k}}| = \mathbb{1}$

$$\Rightarrow \sum_{m:\, \varepsilon_m > E_F} |u_{m\vec{k}} \times u_{m\vec{k}}| = \mathbb{1} - \sum_{m:\, \varepsilon_m < E_F} |u_{m\vec{k}} \times u_{m\vec{k}}|$$

Survives $\qquad = 0$

$$\Rightarrow \sigma_{xy} = -i\hbar \sum_{\substack{n \\ \varepsilon_n < E_F}} \int_{T^2} \frac{d^2k}{(2\pi)^4} \left\{ \langle \tilde{\partial}_y u_{n\vec{k}} | \tilde{\partial}_x u_{n\vec{k}} \rangle - \langle \tilde{\partial}_x u_{n\vec{k}} | \tilde{\partial}_y u_{n\vec{k}} \rangle \right\} \quad (1)$$

9. a) Define the Berry connection of band n:

$$\mathcal{A}_i^{[n]}(\vec{k}) = -i \langle u_{n\vec{k}} | \tilde{\partial}_i u_{n\vec{k}} \rangle$$

$\vec{r} \mapsto \vec{k}$

$\mathcal{M} \mapsto T^2 \; BZ$

$H(\vec{r}) \mapsto \tilde{H}_0(\vec{k})$

$|v(\vec{r})\rangle \mapsto |u_{n\vec{k}}\rangle$

$V(\vec{r}) \mapsto \mathrm{Span}\{|u_{n\vec{k}}\rangle\}$

$n = 1, \quad k = 2$

b) Berry curvature of band n:

$$\mathcal{F}_{ij}^{[n]}(\vec{k}) = \tilde{\partial}_j \mathcal{A}_i^{[n]} - \tilde{\partial}_i \mathcal{A}_j^{[n]}$$

$$= -i \langle \tilde{\partial}_j u_{n\vec{k}} | \tilde{\partial}_i u_{n\vec{k}} \rangle + i \langle \tilde{\partial}_i u_{n\vec{k}} | \tilde{\partial}_j u_{n\vec{k}} \rangle$$

c) → Chern number of band n:

$$C^{[n]} = -\frac{1}{2\pi} \int_{T^2} \mathcal{F}_{xy} \, d^2k = \frac{i}{2\pi} \int_{T^2} \left\{ \langle \tilde{\partial}_y u_{n\vec{k}} | \tilde{\partial}_x u_{n\vec{k}} \rangle - \langle \tilde{\partial}_x u_{n\vec{k}} | \tilde{\partial}_y u_{n\vec{k}} \rangle \right\} d^2k \qquad (2)$$

10. (1) + (2) $\rightarrow$

TKNN formula:

$$\sigma_{xy} = -\frac{e^2}{2\pi\hbar} \sum_{n:\,\varepsilon_n < E_F} C^{[n]} = -\frac{e^2 \nu}{2\pi\hbar}$$

with $\nu = \sum_{n:\,\varepsilon_n < E_F} C^{[n]} \in \mathbb{Z}$

Note:

$$\sigma = \sigma_s + \sigma_a$$

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix}$$

$$\vec{J} = \sigma \vec{E}$$

$$P = \vec{J} \cdot \vec{E}$$

$$P = \vec{E}^T \sigma \vec{E} = \vec{E}^T \sigma_s \vec{E}$$

$\sigma \to \sigma_s + \sigma_a$
