Preparing for calculating the Hall conductivity:
the Kubo formula

1920-1995

Consider a one-particle Hamiltonian H_0 governing a non-interacting many-particle system, e.g. $H_0 = \frac{1}{2m}(\mathbf{p}+e\mathbf{A})^2$ for 2D electrons in a magnetic field

Add a perturbation, e.g. an electric field $\vec{E}(t) = -\frac{\partial \vec{A}}{\partial t}$, choosing a gauge with $\phi = 0$.

New Hamiltonian $H = H_0 + \Delta H$

$$\Delta H = -\vec{J}\cdot\vec{A} \qquad (1)$$

$J_\mu = (q, -\vec{J})$ is a conserved $U(1)$ current, $\partial_\mu J^\mu = 0$, which couples to the source $A^\mu = (\phi, \vec{A})$ as $J_\mu A^\mu$.

To compute the DC current $<\boldsymbol{J}>$ resulting from the added electric field, take $\vec{E}(t) = \vec{E}\, e^{-i\omega t}$ and then take $\omega \to 0$.

We then have $\vec{A} = \frac{\vec{E}}{i\omega} e^{-i\omega t} \qquad (2)$

Working in the interaction picture, operators evolve in time as

$$\mathcal{O}(t) = e^{iH_0 t/\hbar}\, \mathcal{O}\, e^{-iH_0 t/\hbar} \qquad (3)$$

while states evolve as

$$|\Psi(t)\rangle = \mathcal{U}(t, t_0)\, |\Psi(t_0)\rangle \qquad (4)$$

with time evolution operator

$$\mathcal{U}(t, t_0) = \underbrace{T}_{\text{time ordering}} \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \Delta H(t')\, dt'\right) \qquad (5)$$

Prepare the system at time $t \longrightarrow -\infty$ in its (many-body) ground state $|0\rangle$
Then, writing $\mathcal{U}(t) \equiv \mathcal{U}(t, t_0 \rightarrow -\infty)$

$$\begin{aligned}
\langle \mathbf{J}(t)\rangle &= \langle 0(t)|\, \mathbf{J}(t) |0(t)\rangle \\
&= \langle 0| U^{-1}(t) \mathbf{J}(t) U(t)\, |0\rangle \\
&\approx \langle 0| \left(\cancel{\mathbf{J}(t)} + \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, [\Delta H(t'), \mathbf{J}(t)]\right) |0\rangle \qquad (6)
\end{aligned}$$

current in the absence of an electric field vanishes

keep only leading terms in the expansions of $\mathcal{U}$ and $\mathcal{U}^{-1}$ ($\Rightarrow$ don't have to worry about time ordering)

* Note :
no contribution from $[A_j(t'), J_i(t)]$ since we treat $\vec{E}(t')$ as a classical field (not an operator).

Using (1) and (2)

$$\langle J_i(t)\rangle = \frac{1}{\hbar\omega}\int_{-\infty}^{t} dt'\, \langle 0|\underbrace{[J_j(t'), J_i(t)]}_{[J_j(0),\, J_i(t-t')]}|0\rangle\, E_j\, e^{-i\omega t'} \qquad (7)^{*}$$

Invariance under time translations: the correlation function in the integrand can only depend on $t'' = t - t'$. We can then write

$$\langle J_i(t)\rangle = \frac{1}{\hbar\omega}\left(\int_0^{\infty} dt''\, e^{i\omega t''}\, \langle 0|[J_j(0), J_i(t'')]|0\rangle\right) E_j e^{-i\omega t} \qquad (8)$$

Note that the current responds by oscillating at the same frequency as the perturbation (the electric field). Linear response!

$\Downarrow$

Hall conductivity

$$\sigma_{xy}(\omega) = \frac{1}{\hbar\omega}\int_0^{\infty} dt\, e^{i\omega t}\, \langle 0|[J_y(0), J_x(t)]|0\rangle \qquad (9)$$

$\Downarrow$ use that $\vec{J}(t) = e^{iH_0 t/\hbar}\, \vec{J}(0)\, e^{-iH_0 t/\hbar}$ and insert a complete set of eigenstates $\{|n\rangle\}$ of H_0

$$\sigma_{xy}(\omega) = \frac{1}{\hbar\omega}\int_0^{\infty} dt\, e^{i\omega t} \sum_n \left[\langle 0|J_y|n\rangle\langle n|J_x|0\rangle e^{i(E_n-E_0)t/\hbar} - \langle 0|J_x|n\rangle\langle n|J_y|0\rangle e^{i(E_0-E_n)t/\hbar}\right] \qquad (10)$$

Performing the integral and noticing that states with |*n*> = |*0*> don't contribute:

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

Binomial expansion:

$$\frac{1}{\hbar\omega + E_n - E_0} \approx \frac{1}{E_n - E_0} - \frac{\hbar\omega}{(E_n - E_0)^2} + \mathcal{O}(\omega^2)\ldots$$

and similar for the other term.

The leading term in the expansion of (11) (which looks divergent in the w —> 0 limit!) vanishes due to rotational invariance under *x* —> *y*, *y* —> –*x* (cf. the antisymmetry of the Hall conductivity in the Drude formalism)

We're then left with

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

Kubo formula for the Hall conductivity

in the w —> 0 limit.

Doing algebra on the Kubo formula with Bloch states:

(using a "lazy" notation ... the bands come with separate momentum integrals, and not a single integral ... but the end result will be the same)

$$\sigma_{xy} = i\hbar \sum_{E_\alpha < E_F < E_\beta} \int_{\mathbf{T}^2} \frac{d^2k}{(2\pi)^2} \frac{\langle u^\alpha_{\mathbf{k}}|J_y|u^\beta_{\mathbf{k}}\rangle\langle u^\beta_{\mathbf{k}}|J_x|u^\alpha_{\mathbf{k}}\rangle - \langle u^\alpha_{\mathbf{k}}|J_x|u^\beta_{\mathbf{k}}\rangle\langle u^\beta_{\mathbf{k}}|J_y|u^\alpha_{\mathbf{k}}\rangle}{(E_\beta(\mathbf{k}) - E_\alpha(\mathbf{k}))^2} \qquad (14)$$

$$\mathbf{J} = \frac{e}{\hbar}\frac{\partial \tilde{H}}{\partial \mathbf{k}} \quad \text{where} \quad \tilde{H}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{x}} H e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{with} \quad H|\psi_{\mathbf{k}}\rangle = E_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle \qquad (15)$$

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_{E_\alpha < E_F < E_\beta} \int_{\mathbf{T}^2} \frac{d^2k}{(2\pi)^2} \frac{\langle u^\alpha_{\mathbf{k}}|\partial_y\tilde{H}|u^\beta_{\mathbf{k}}\rangle\langle u^\beta_{\mathbf{k}}|\partial_x\tilde{H}|u^\alpha_{\mathbf{k}}\rangle - \langle u^\alpha_{\mathbf{k}}|\partial_x\tilde{H}|u^\beta_{\mathbf{k}}\rangle\langle u^\beta_{\mathbf{k}}|\partial_y\tilde{H}|u^\alpha_{\mathbf{k}}\rangle}{(E_\beta(\mathbf{k}) - E_\alpha(\mathbf{k}))^2} \qquad (16)$$

$$\begin{aligned}
\langle u^\alpha_{\mathbf{k}}|\partial_i\tilde{H}|u^\beta_{\mathbf{k}}\rangle &= \langle u^\alpha_{\mathbf{k}}|\partial_i\left(\tilde{H}|u^\beta_{\mathbf{k}}\rangle\right) - \langle u^\alpha_{\mathbf{k}}|\tilde{H}|\partial_i u^\beta_{\mathbf{k}}\rangle \\
&= (E_\beta(\mathbf{k}) - E_\alpha(\mathbf{k}))\langle u^\alpha_{\mathbf{k}}|\partial_i u^\beta_{\mathbf{k}}\rangle \\
&= -(E_\beta(\mathbf{k}) - E_\alpha(\mathbf{k}))\langle \partial_i u^\alpha_{\mathbf{k}}|u^\beta_{\mathbf{k}}\rangle
\end{aligned}$$

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_{E_\alpha < E_F < E_\beta} \int_{\mathbf{T}^2} \frac{d^2k}{(2\pi)^2} \langle \partial_y u^{\alpha}_{\mathbf{k}} | u^{\beta}_{\mathbf{k}} \rangle \langle u^{\beta}_{\mathbf{k}} | \partial_x u^{\alpha}_{\mathbf{k}} \rangle - \langle \partial_x u^{\alpha}_{\mathbf{k}} | u^{\beta}_{\mathbf{k}} \rangle \langle u^{\beta}_{\mathbf{k}} | \partial_y u^{\alpha}_{\mathbf{k}} \rangle \quad (17)$$

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_{\alpha} \int_{\mathbf{T}^2} \frac{d^2k}{(2\pi)^2} \langle \partial_y u^{\alpha}_{\mathbf{k}} | \partial_x u^{\alpha}_{\mathbf{k}} \rangle - \langle \partial_x u^{\alpha}_{\mathbf{k}} | \partial_y u^{\alpha}_{\mathbf{k}} \rangle \quad (18)$$

$$\mathcal{F}_{xy} = \frac{\partial \mathcal{A}_x}{\partial k^y} - \frac{\partial \mathcal{A}_y}{\partial k^x} = -i \left\langle \frac{\partial u}{\partial k^y} \middle| \frac{\partial u}{\partial k^x} \right\rangle + i \left\langle \frac{\partial u}{\partial k^x} \middle| \frac{\partial u}{\partial k^y} \right\rangle$$

$$C = -\frac{1}{2\pi} \int_{\mathbf{T}^2} d^2k \, \mathcal{F}_{xy}$$

$$\sigma_{xy} = -\frac{e^2}{2\pi\hbar} \sum_{\alpha} C_\alpha \quad (19)$$

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