Fundamentals of dc conductivity:
Longitudinal and transverse

Raffaele Resta

Trieste, 2023

Linear conductivity

$$\sigma_{\alpha\beta}(\omega) = \frac{\partial j_\alpha(\omega)}{\partial \mathcal{E}_\beta(\omega)}$$

- The conductivity tensor $\sigma_{\alpha\beta}(\omega)$ is partitioned into its symmetric and antisymmetric components:

$$\begin{aligned} j_\alpha(\omega) &= \sigma^{(+)}_{\alpha\beta}(\omega)\,\mathcal{E}_\beta(\omega) && \text{longitudinal} \\ j_\alpha(\omega) &= \sigma^{(-)}_{\alpha\beta}(\omega)\,\mathcal{E}_\beta(\omega) && \text{Hall (transverse)} \end{aligned}$$

- Focus here on **dc conductivity**:

$$\text{Re } \sigma_{\alpha\beta}(\omega) \text{ at } \omega = 0$$

- Re $\sigma^{(\pm)}_{\alpha\beta}(\omega)$ related to Im $\sigma^{(\pm)}_{\alpha\beta}(\omega)$ (Kramers-Kronig)

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Motivation

- **Linear** Hall conductivity requires breaking of T-symmetry:
  - **Normal:** T-symmetry broken by an applied **B** field
  - **Anomalous:** T-symmetry spontaneously broken (e.g. in ferromagnets)

- T-symmetry does not forbid **nonlinear Hall** conductivity:

  I. Sodemann & L. Fu,
  Quantum Nonlinear Hall Effect Induced by Berry Curvature Dipole in Time-Reversal Invariant Materials,
  Phys. Rev. Lett. 2015

- **Everything you always wanted to know about dc conductivity (but were afraid to ask):**

  Theory of longitudinal and transverse nonlinear dc conductivity,
  Phys. Rev. Research **4**, 033002 (2022)

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Outline

1. Longitudinal conductivity, linear
   - Classical theory
   - Quantum theory
   - Boundary conditions

2. Adiabatic electron transport

3. Kohn's approach to linear dc conductivity

4. Anomalous Hall conductivity (linear)

5. Independent-electron formulation in a crystalline material

6. Appendix: Many-body Chern number

Outline

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Classical Drude theory

P. Drude, Annalen der Physik. **306**, 566 (1900)

- From **Ashcroft-Mermin, Chapter 1**:
  (dissipation enters the EOM **directly** via a relaxation time τ)

$$\sigma_{\text{Drude}}(\omega) = \frac{ie^2}{\omega + i/\tau}\left(\frac{n}{m}\right), \qquad \frac{n}{m} = \frac{\text{electron density}}{\text{electron mass}}$$

$$\sigma_{\text{Drude}}(0) = \tau e^2 \left(\frac{n}{m}\right) \qquad \text{Ohm's law}$$

- In the nondissipative $\tau \to \infty$ limit:

$$\sigma_{\text{Drude}}(\omega) = D_{\text{classical}}\left[\delta(\omega) + \frac{i}{\pi\omega}\right] \qquad D_{\text{classical}} = \pi e^2 \frac{n}{m}$$

- Real and imaginary parts related by Kramers-Kronig

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- In a macroscopic field $\mathcal{E}$ the electrons undergo free-acceleration
- Classical case:
  - The electronic **inverse inertia** is measured by $D_{\text{classical}}$
- QM case:
  - The inverse inertia of the many-electron system is measured by a tensor $D_{\alpha\beta}$: **Drude weight** a.k.a. charge sfiffness
  - Interacting electron gas in a **flat potential**: $D_{\alpha\beta} = D_{\text{classical}}\, \delta_{\alpha\beta}$
  - In a crystalline potential $D_{\alpha\beta} \neq D_{\text{classical}}\, \delta_{\alpha\beta}$

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A simple exercise: classical Drude formula in 1d

Alternative derivation in the **vector-potential gauge**:

$$\mathcal{E}(t) = -\frac{1}{c}\frac{dA(t)}{dt}$$

- Free-electron Hamiltonian:

$$H = \frac{1}{2m}\left[p + \frac{e}{c}A(t)\right]^2$$

- Velocity:

$$v(t) = \frac{1}{m}\left[p + \frac{e}{c}A(t)\right]$$

- Current density:

$$j(t) = -\frac{en}{m}\left[p + \frac{e}{c}A(t)\right]$$

$$j(\omega) = -\frac{e^2 n}{mc}A(\omega) = -\frac{D_{\text{classical}}}{\pi c}A(\omega)$$

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- $A(\omega)$ in function of $\mathcal{E}(\omega)$:

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Naive inversion: $A(\omega) = -\frac{ic}{\omega}\mathcal{E}(\omega)$????

Wrong! The inversion is $A(\omega) = -c\left(\frac{i}{\omega} + \text{const} \times \delta(\omega)\right)\mathcal{E}(\omega)$

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- Multiplying the two factors:

$$\begin{aligned}\sigma_{\text{Drude}}(\omega) &= \frac{dj(\omega)}{dA(\omega)}\frac{dA(\omega)}{d\mathcal{E}(\omega)} \\ &= -\frac{e^2 n}{mc} \times -c\left[\pi\delta(\omega) + \frac{i}{\omega}\right] \\ &= D_{\text{classical}}\left[\delta(\omega) + \frac{i}{\pi\omega}\right]\end{aligned}$$

- **Key message:**
  - Drude weight = derivative of **j** wrt to **A**
  - ω-dependent factor = derivative of **A** wrt $\mathcal{E}$

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Outline

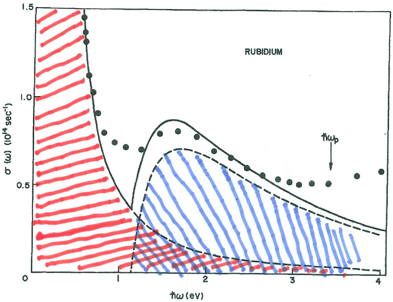
Drude & regular terms in a real metal

- The Drude weight still measures the many-electron **free acceleration**:

$$\sigma^{(+)}_{\alpha\beta}(\omega) = \sigma^{(\mathrm{Drude})}_{\alpha\beta}(\omega) + \sigma^{(\mathrm{regular})}_{\alpha\beta}(\omega)$$
$$= D_{\alpha\beta}\left[\delta(\omega) + \frac{i}{\pi\omega}\right] + \sigma^{(\mathrm{regular})}_{\alpha\beta}(\omega)$$

$\sigma(\omega)$ in Rubidium

- **Dots:** experiment (N. V. Smith, 1970)
- **Red:** Drude (broadened by **extrinsic** effects)
- **Blue:** Regular
- **Solid:** sum of the two terms



f-sum rule

- Interacting electron gas in a flat potential:

$$\sigma^{(\text{regular})}_{\alpha\beta}(\omega) = 0, \qquad D_{\alpha\beta} = D_{\text{classical}}\delta_{\alpha\beta}$$

- After switching on the crystalline potential:

$$\sigma^{(+)}_{\alpha\beta}(\omega) = D_{\alpha\beta}\left[\delta(\omega) + \frac{i}{\pi\omega}\right] + \sigma^{(\text{regular})}_{\alpha\beta}(\omega)$$

- The two terms are related by the f-sum rule

$$\int_0^\infty d\omega \ \text{Re}\ \sigma_{\alpha\beta}(\omega) = \frac{D_{\alpha\beta}}{2} + \int_0^\infty d\omega \ \text{Re}\ \sigma^{(\text{regular})}_{\alpha\beta}(\omega) = \frac{D_{\text{classical}}}{2}\delta_{\alpha\beta}$$

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Ground-state vs. dynamical properties

- Switching on the crystalline potential transfers some spectral weight from $\sigma^{(\mathrm{Drude})}_{\alpha\beta}(\omega)$ to $\sigma^{(\mathrm{regular})}_{\alpha\beta}(\omega)$
- In insulators $D_{\alpha\beta} = 0$

- $\sigma^{(\mathrm{regular})}_{\alpha\beta}(\omega)$ is a **dynamical** property
(it requires sum-over-states Kubo formulæ)
- $D_{\alpha\beta}$ is a **ground-state** property
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- **All dc conductivities** are ground-state properties:
Longitudinal & transverse, linear & nonlinear

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Effective electron density

- The Drude weight measures the inverse inertia of the many-electron system
- Switching on the crystalline potential:

$$D_{\text{classical}}\, \delta_{\alpha\beta} = \frac{\pi e^2}{m} n\, \delta_{\alpha\beta} \qquad \Longrightarrow \qquad D_{\alpha\beta} = \frac{\pi e^2}{m} n^*_{\alpha\beta}$$

- The periodic potential **hinders** the free acceleration

$$n^*_{\alpha\alpha} \qquad < \qquad n$$

- Effective electron density contributing to the dc current:

$$n^*_{\alpha\beta} = \frac{m}{\pi e^2} D_{\alpha\beta}$$

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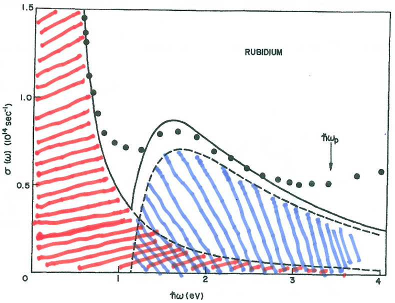
f-sum rule revisited

$$\frac{D_{\alpha\beta}}{2} + \int_0^\infty d\omega \ \mathrm{Re}\ \sigma_{\alpha\beta}^{(\text{regular})}(\omega) = \frac{\pi e^2 n}{2m}\delta_{\alpha\beta}$$

$$n^*_{\alpha\beta} + \frac{2m}{\pi e^2}\int_0^\infty d\omega \ \mathrm{Re}\ \sigma_{\alpha\beta}^{(\text{regular})}(\omega) = n\,\delta_{\alpha\beta}$$

For a given electron density n:

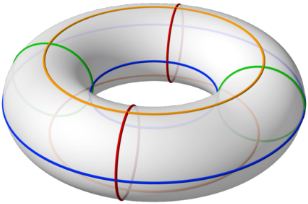
- **In a flat potential:** Only the Drude peak, $\sigma_{\alpha\beta}^{(\text{regular})}(\omega) = 0$
- **In crystalline metals:** Both terms are nonzero
- **In insulators:** Only the regular term, $D_{\alpha\beta} = 0$



Outline

Schrödinger equation in condensed matter

- Periodic vs. “open”



Born-von-Kàrmàn PBCs
(toroidal)

Open boundary conditions
(bounded crystallite)

- **Closed circuit:**
  PBCs are the natural framework for conductivity
  but also for condensed matter theory in general
- **Open circuit:**
  No dc current may flow in a bounded crystallite

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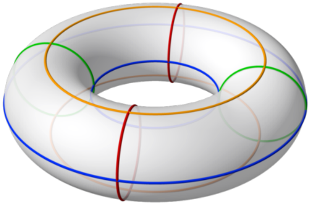

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Drude weight within open boundary conditions

G. Bellomia & R. Resta, Phys. Rev. b **102**, 205123 (2020)

- Is it possible to compute D by solving Schrödinger equation for the many-electron system within OBCs?

- **Yes!**
  The inverse inertia can be probed in a different way

- **How?**
  From the linear response to a low-frequency $\mathcal{E}(\omega)$

- The system (bounded crystallite) has normal modes which coalesce to $\omega = 0$ in the $1/L$ limit

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The problem

- Hamiltonian depending on two parameters (t-independent)

$$\hat{H} = \hat{H}_{\kappa_1,\kappa_2} \qquad |\Psi_0\rangle \text{ and } E_0 \text{ also depend on } (\kappa_1, \kappa_2)$$

- Focus on an operator $\hat{O}$ which can be written as

$$\hat{O} = \partial_{\kappa_1} \hat{H} \qquad \text{derivative wrt the first parameter}$$

- Ground-state expectation value

$$\langle \hat{O} \rangle = \langle \Psi_0 | \hat{O} | \Psi_0 \rangle = \partial_{\kappa_1} E_0 \qquad \text{Hellmann-Feynman}$$

- When $\hat{H}$ is varied in time: $\hat{H} \Rightarrow \hat{H}(t)$

$$\langle \hat{O}(t) \rangle = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle = ????$$

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Niu-Thouless theorem (1984)

- The time-dependence of $\hat{H}$ occurs via $\kappa_2 \Rightarrow \kappa_2(t)$:

$$\hat{H}(t) = \hat{H}_{\kappa_1,\kappa_2(t)}, \qquad \hat{H}(t)|\Psi(t)\rangle = i\hbar\frac{d}{dt}|\Psi(t)\rangle$$

- In the adiabatic limit:

$$\langle\hat{O}(t)\rangle = \partial_{\kappa_1}E_0 - \hbar\,\Omega(\kappa_1,\kappa_2)\dot{\kappa}_2(t)$$

$$\Omega(\kappa_1,\kappa_2) = i\left(\langle\partial_{\kappa_1}\Psi_0|\partial_{\kappa_2}\Psi_0\rangle - \langle\partial_{\kappa_2}\Psi_0|\partial_{\kappa_1}\Psi_0\rangle\right)$$

- Main features of the Niu-Thouless formula:
  - $\Omega(\kappa_1,\kappa_2)$ is called today a **Berry curvature**
  - Both $\partial_{\kappa_1}E_0$ and $\Omega(\kappa_1,\kappa_2)$ depend implicitly on time
  - Exact for **infinitesimal** $\dot{\kappa}_2(t)$ (i.e. in the adiabatic limit)
  - It converges to Hellmann-Feynman for $\dot{\kappa}_2(t) \to 0$

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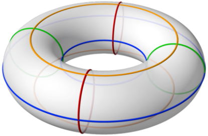
$$\Omega(\kappa_1,\kappa_2) = i\left(\langle\partial_{\kappa_1}\Psi_0|\partial_{\kappa_2}\Psi_0\rangle - \langle\partial_{\kappa_2}\Psi_0|\partial_{\kappa_1}\Psi_0\rangle\right)$$

- Main features of the Niu-Thouless formula:
  - $\Omega(\kappa_1,\kappa_2)$ is called today a **Berry curvature**
  - Both $\partial_{\kappa_1}E_0$ and $\Omega(\kappa_1,\kappa_2)$ depend implicitly on time
  - Exact for **infinitesimal** $\dot{\kappa}_2(t)$ (i.e. in the adiabatic limit)
  - It converges to Hellmann-Feynman for $\dot{\kappa}_2(t) \to 0$

Outline

Kohn's Hamiltonian (1964)



$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m}\sum_{i=1}^{N}\left[\mathbf{p}_i + \frac{e}{c}\mathbf{A}^{(\mathrm{micro})}(\mathbf{r}_i) + \hbar\boldsymbol{\kappa}\right]^2 + \hat{V}$$

- N-electron $|\Psi_0\rangle$ depending on $\boldsymbol{\kappa} = (\kappa_x, \kappa_y, \kappa_z)$
- Born-von-Kàrmàn **PBCs** over a period L:
  The coordinates $r_{i\alpha}$ are actually **angles** $\varphi_{i\alpha} = 2\pi r_{i\alpha}/L$
- $\hat{V}$ one-body (possibly disordered) and two-body potentials
- $\mathbf{A}^{(\mathrm{micro})}(\mathbf{r}_i)$ needed to break T-symmetry
- $\boldsymbol{\kappa}$-derivatives taken first, $L \to \infty$ limit after

The 3d parameter $\boldsymbol{\kappa} = (\kappa_x, \kappa_y, \kappa_z)$

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m} \sum_{i=1}^{N} \left[\mathbf{p}_i + \frac{e}{c} \mathbf{A}^{(\text{micro})}(\mathbf{r}_i) + \hbar \boldsymbol{\kappa} \right]^2 + \hat{V}$$

- $\boldsymbol{\kappa}$ "flux" or "twist" (dimensions: inverse length)
- Equivalent to an additional vector potential

$$\hbar \boldsymbol{\kappa} \equiv \frac{e}{c} \mathbf{A} \qquad \{\mathbf{r}_i\}\text{-independent}$$

- Two different cases
  1. t-independent $\boldsymbol{\kappa}$: a pure **gauge-transformation**
  2. t-dependent $\boldsymbol{\kappa}$: **macroscopic field**

$$\mathcal{E}(t) = -\frac{\hbar}{e} \dot{\boldsymbol{\kappa}}(t)$$

The operator $\hat{O}$: macroscopic current density

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m} \sum_{i=1}^{N} \left[\mathbf{p}_i + \frac{e}{c} \mathbf{A}^{(\text{micro})}(\mathbf{r}_i) + \hbar \boldsymbol{\kappa} \right]^2 + \hat{V}$$

- Many-body velocity operator (extensive):

$$\hat{\mathbf{v}} = \frac{1}{m} \sum_{i=1}^{N} \left[\mathbf{p}_i + \frac{e}{c} \mathbf{A}^{(\text{micro})}(\mathbf{r}_i) + \hbar \boldsymbol{\kappa} \right] = \frac{1}{\hbar} \partial_{\boldsymbol{\kappa}} \hat{H}_{\boldsymbol{\kappa}}$$

- Macroscopic current-density operator:

$$\hat{\mathbf{j}} = -\frac{e}{\hbar L^3} \partial_{\boldsymbol{\kappa}} \hat{H}_{\boldsymbol{\kappa}}$$

- Niu-Thouless formula:

$$\langle \hat{j}_\alpha(t) \rangle = -\frac{e}{\hbar L^3} [\, \partial_{\kappa_\alpha} E_0 - \hbar\, \Omega(\kappa_\alpha, \kappa_\beta) \dot{\kappa}_\beta(t) \,]$$

Berry curvature

- Berry curvature (change of notation):

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa}) \equiv \Omega(\kappa_\alpha, \kappa_\beta) = i\left(\langle \partial_{\kappa_1}\Psi_0 | \partial_{\kappa_2}\Psi_0\rangle - \langle \partial_{\kappa_2}\Psi_0 | \partial_{\kappa_1}\Psi_0\rangle\right)$$

- Niu-Thouless formula:

$$\begin{aligned} j_\alpha(t) &= \langle \hat{j}_\alpha(t)\rangle = -\frac{e}{\hbar L^3}\left[\partial_{\kappa_\alpha} E_0 - \hbar\,\Omega_{\alpha\beta}(\boldsymbol{\kappa})\dot{\kappa}_\beta(t)\right] \\ &= 0 \qquad \text{if } \boldsymbol{\kappa}(t) \equiv 0 \end{aligned}$$

- Symmetry properties:
  - In presence of **T-symmetry** $\Omega_{\alpha\beta}(\boldsymbol{\kappa}) = -\Omega_{\alpha\beta}(-\boldsymbol{\kappa})$
  - In presence of **I-symmetry** $\Omega_{\alpha\beta}(\boldsymbol{\kappa}) = \Omega_{\alpha\beta}(-\boldsymbol{\kappa})$
  - $\Omega_{\alpha\beta}(0) \neq 0$ needs **time-reversal** symmetry broken

Case 1: t-independent flux, longitudinal conductivity

- Current induced by a constant vector potential:

$$\left.\frac{\partial j_\alpha(t)}{\partial \kappa_\beta}\right|_{\boldsymbol{\kappa}=0} = -\frac{\partial}{\partial \kappa_\beta} \frac{e}{\hbar L^3} \frac{\partial E_0}{\partial \kappa_\alpha}$$

time-independent

$$\frac{\partial j_\alpha}{\partial A_\beta} = \frac{e}{\hbar c} \frac{\partial j_\alpha}{\partial \kappa_\beta} = -\frac{e^2}{\hbar^2 c L^3} \frac{\partial^2 E_0}{\partial \kappa_\alpha \partial \kappa_\beta}$$

- A constant vector potential is a pure gauge: why is E_0 **gauge-dependent ?**
- Born-von-Kàrmàn PBCs **violate** gauge-invariance

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Longitudinal conductivity

- The chain rule

$$\sigma_{\alpha\beta}(\omega) = \frac{\partial j_\alpha(\omega)}{\partial \mathcal{E}_\beta(\omega)} = \frac{\partial j_\alpha(\omega)}{\partial A_\beta(\omega)} \frac{dA(\omega)}{d\mathcal{E}(\omega)}$$

  - $dA(\omega)/d\mathcal{E}(\omega)$ same as in the **classical** case
  - $\partial j_\alpha(\omega)/\partial A_\beta(\omega)$ requires sum-over-states Kubo formula

- In the **dc** case: response to a **static A**

$$\sigma_{\alpha\beta}^{\text{(Drude)}}(\omega) = -\frac{e^2}{\hbar^2 c L^3} \frac{\partial^2 E_0}{\partial\kappa_\alpha \partial\kappa_\beta} \times -c \left[\pi\delta(\omega) + \frac{i}{\omega}\right]$$

$$= D_{\alpha\beta}\left[\delta(\omega) + \frac{i}{\pi\omega}\right] \qquad D_{\alpha\beta} = \frac{\pi e^2}{\hbar^2 L^3} \frac{\partial^2 E_0}{\partial\kappa_\alpha \partial\kappa_\beta}$$

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The famous Kohn's formula (1964)

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Outline

Case 2: time-dependent flux (adiabatically)

- Constant $\mathcal{E}$ field $\Rightarrow$ $\boldsymbol{\kappa}$ linear in time

$$\mathcal{E} = -\frac{1}{c}\frac{d\mathbf{A}(t)}{dt}, \qquad \boldsymbol{\kappa} = -\frac{e}{\hbar}\mathcal{E}t$$

- Second term in the Niu-Thouless fomula:

$$\begin{aligned} j_\alpha(t) &= -\frac{e}{\hbar L^3}[\,\partial_{\kappa_\alpha} E_0 - \hbar\,\Omega_{\alpha\beta}(\boldsymbol{\kappa})\dot{\kappa}_\beta(t)\,] \\ &= -\frac{e^2}{\hbar L^3}\,\Omega_{\alpha\beta}(\boldsymbol{\kappa})\mathcal{E}_\beta \qquad \text{time independent at } \boldsymbol{\kappa} = 0 \end{aligned}$$

  - The extra term yields a dc current: no **dissipation** needeed
  - The is current **normal** to the field: $\Omega_{\alpha\beta}(\boldsymbol{\kappa})$ **antisymmetric**
  - It could be nonzero even in **insulators**

- Bottom line: **anomalous Hall conductivity** (linear):

$$\sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar L^3}\,\Omega_{\alpha\beta}(0)$$

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Linear anomalous Hall conductivity: Summary

- Linear Hall conductivity: **Geometric term** (in insulators and metals, in 2*d* and 3*d*)

$$\sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar L^d}\Omega_{\alpha\beta}(0) \qquad \text{in the } L \to \infty \text{ limit}$$

- Many-body Berry curvature (extensive):

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa}) = i\,(\,\langle \partial_{\kappa_\alpha}\Psi_0 | \partial_{\kappa_\beta}\Psi_0\rangle - \langle \partial_{\kappa_\alpha}\Psi_0 | \partial_{\kappa_\beta}\Psi_0\rangle\,)$$

- $\Omega_{\alpha\beta}(0) \neq 0$ only if **T** symmetry is broken

- **Extrinsic** terms always present in **metals**

- Topological in 2*d* **insulators** (Niu, Thouless, & Wu, 1985): extrinsic effects irrelevant

Outline

Band structure (Hartree-Fock or Kohn-Sham)

- The many-body ground state $|\Psi_0\rangle$:
  Slater determinant of Bloch orbitals (doubly occupied)
  $|\psi_{j\mathbf{k}}\rangle = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}|u_{j\mathbf{k}}\rangle$ with energy $\epsilon_{j\mathbf{k}}$

- In the $L \to \infty$ limit **k** is a continuous variable

- Intensive ground state observables are **k**-integrals:
  - Over the **Brillouin zone** (insulators)
  - Over the **Fermi volume** (metals)

- Example: band energy per unit volume

$$\frac{E_0}{L^d} \quad \Longrightarrow \quad 2\sum_j \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d}\, f(\mu - \epsilon_{j\mathbf{k}})\, \epsilon_{j\mathbf{k}}, \quad \mu = \text{Fermi level}$$

Longitudinal conductivity

- Kohn's Drude weight

$$D_{\alpha\beta} = \frac{\pi e^2}{\hbar^2 L^3} \frac{\partial^2 E_0}{\partial\kappa_\alpha \partial\kappa_\beta} \qquad \text{at } \boldsymbol{\kappa} = 0$$

$$\Longrightarrow \quad 2\pi e^2 \sum_j \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \, f(\mu - \epsilon_{j\mathbf{k}}) \, m^{-1}_{j,\alpha\beta}(\mathbf{k})$$

$$m^{-1}_{j,\alpha\beta}(\mathbf{k}) = \frac{1}{\hbar^2} \frac{\partial^2 \epsilon_{j\mathbf{k}}}{\partial k_\alpha \partial k_\beta} \qquad \text{inverse effective mass of band } j$$

- Integrating by parts:
  Fermi volume integral $\Rightarrow$ **Fermi surface** integral

- Landau's Fermi-liquid theory:
  Charge transport involves only quasiparticles with energies within $k_{\mathrm{B}} T$ from the Fermi level

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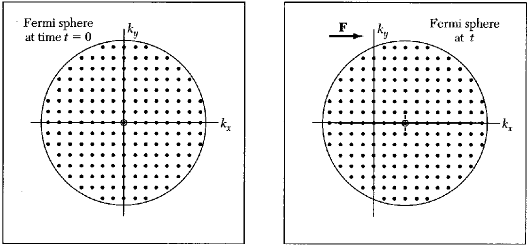
Charge transport as an "intraband" property



- Fermi-volume to Fermi-surface (integrating by parts):

$$D_{\alpha\beta} = \frac{2\pi e^2}{\hbar^2} \sum_j \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \, f(\mu - \epsilon_{j\mathbf{k}}) \frac{\partial^2 \epsilon_{j\mathbf{k}}}{\partial k_\alpha \partial k_\beta}$$

$$= -2\pi e^2 \sum_j \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \, f'(\epsilon_{j\mathbf{k}}) \, v_{j\alpha}(\mathbf{k}) v_{j\beta}(\mathbf{k}), \quad v_{j\alpha}(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \epsilon_{j\mathbf{k}}}{\partial k_\alpha}$$

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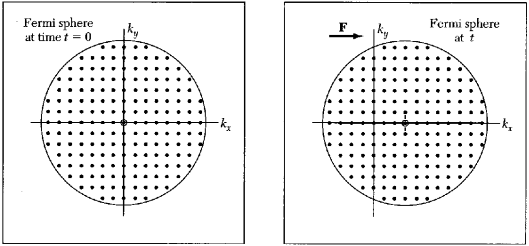

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$$
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&= -2\pi e^2 \sum_j \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} \; f'(\epsilon_{j\mathbf{k}}) \; v_{j\alpha}(\mathbf{k}) v_{j\beta}(\mathbf{k}), \quad v_{j\alpha}(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \epsilon_{j\mathbf{k}}}{\partial k_\alpha}
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$$

Anomalous Hall conductivity (linear)

- Berry curvature of band j:

$$\tilde{\Omega}_{j,\alpha\beta}(\mathbf{k}) = i\,(\,\langle \partial_{k_\alpha} u_{j\mathbf{k}} | \partial_{k_\beta} u_{j\mathbf{k}} \rangle - \langle \partial_{k_\beta} u_{j\mathbf{k}} | \partial_{k_\alpha} u_{j\mathbf{k}} \rangle\,)$$

- Many-body Berry curvature at $\boldsymbol{\kappa} = 0$

$$\frac{1}{L^d}\Omega_{\alpha\beta}(0) \quad \Longrightarrow \quad \sum_j \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d}\; f(\mu - \epsilon_{j\mathbf{k}})\; \tilde{\Omega}_{j,\alpha\beta}(\mathbf{k})$$

- Intrinsic Hall conductivity (insulators and metals):

$$\sigma^{(-)}_{\alpha\beta}(0) \qquad \Longrightarrow \qquad -\frac{e^2}{\hbar} \sum_j \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^d}\; f(\mu - \epsilon_{j\mathbf{k}})\; \tilde{\Omega}_{j,\alpha\beta}(\mathbf{k})$$

- Topological in $2d$ insulators:

$$\sigma^{(-)}_{xy}(0) = -\frac{e^2}{\hbar} \sum_{j=\mathrm{occ.}} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2}\; \tilde{\Omega}_{j,xy}(\mathbf{k}) = -\frac{e^2}{h} C_1$$

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Summary

- Generalities about dc conductivity
  (classical & quantum-mechanical)

- Many-body Hamiltonian with a "flux" (Kohn 1964)
  - Linear longitudinal conductivity
  - Lineal Hall conductivity

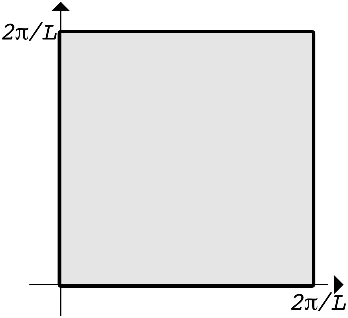
- Bloch theory & band-structure
  - Linear longitudinal conductivity
  - Lineal Hall conductivity

- Appendix: The Niu-Thouless-Wu many-body Chern number

Outline

Integrating the 2*d* many-body Berry curvature

$$\Omega_{xy}(\boldsymbol{\kappa}) = i\,(\,\langle \partial_{\kappa_x} \Psi_{0\boldsymbol{\kappa}} | \partial_{\kappa_y} \Psi_{0\boldsymbol{\kappa}} \rangle - \langle \partial_{\kappa_y} \Psi_{0\boldsymbol{\kappa}} | \partial_{\kappa_x} \Psi_{0\boldsymbol{\kappa}} \rangle\,)$$



$$C_1 = \frac{1}{2\pi} \int_0^{\frac{2\pi}{L}} d\kappa_x \int_0^{\frac{2\pi}{L}} d\kappa_y \; \Omega_{xy}(\boldsymbol{\kappa})$$

The domain is a **torus** if and only if the system is **insulating**

Single-point Chern number

- Chern theorem on a torus:

$$\frac{1}{2\pi}\int_0^{\frac{2\pi}{L}} d\kappa_x \int_0^{\frac{2\pi}{L}} d\kappa_y \; \Omega_{xy}(\boldsymbol{\kappa}) = C_1 \in \mathbb{Z}, \qquad \text{any } L$$

- In the $L \to \infty$ limit:

$$\frac{1}{2\pi}\int_0^{\frac{2\pi}{L}} d\kappa_x \int_0^{\frac{2\pi}{L}} d\kappa_y \; \Omega_{xy}(\boldsymbol{\kappa}) \; \to \; \frac{1}{2\pi}\left(\frac{2\pi}{L}\right)^2 \Omega_{xy}(0) = \frac{2\pi}{L^2}\Omega_{xy}(0)$$

QAHE in 2d insulators

- General formula for linear Hall conductivity, in insulators and metals, in 2d and 3d:

$$\sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar L^d}\Omega_{\alpha\beta}(0) \qquad \text{in the } L \to \infty \text{ limit}$$

- In 2d:

$$\sigma^{(-)}_{xy}(0) = -\frac{e^2}{h}\frac{2\pi}{L^2}\Omega_{xy}(0)$$

- In 2d insulators:

$$\frac{2\pi}{L^2}\Omega_{xy}(0) \to C_1, \qquad \sigma^{(-)}_{xy}(0) \to -\frac{e^2}{h}C_1$$

Niu, Thouless, and Wu, Phys. Rev. B **31**, 3372 (1985)

QAHE in 2*d* insulators

- General formula for linear Hall conductivity, in insulators and metals, in 2*d* and 3*d*:

$$\sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar L^d}\Omega_{\alpha\beta}(0) \qquad \text{in the } L \to \infty \text{ limit}$$

- In 2*d*:

$$\sigma^{(-)}_{xy}(0) = -\frac{e^2}{h}\frac{2\pi}{L^2}\Omega_{xy}(0)$$

- In 2*d* insulators:

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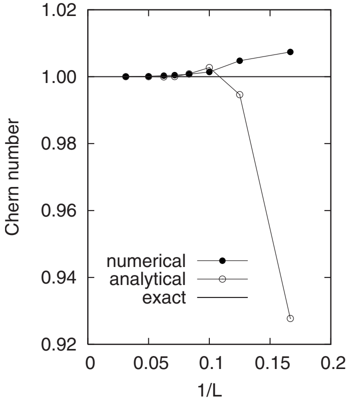
Convergence of the many-body Chern number



$$\frac{2\pi}{L^2}\Omega_{xy}(0) \;\rightarrow\; C_1$$

- Tight-binding simulation (Haldane model Hamiltonian)
  D. Ceresoli & R. Resta, Phys. Rev. B **76**, 012405 (2007)