Adiabaticity and quantum geometry in DFT

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10th Time-Dependent Density-Functional Theory: Prospects and Applications

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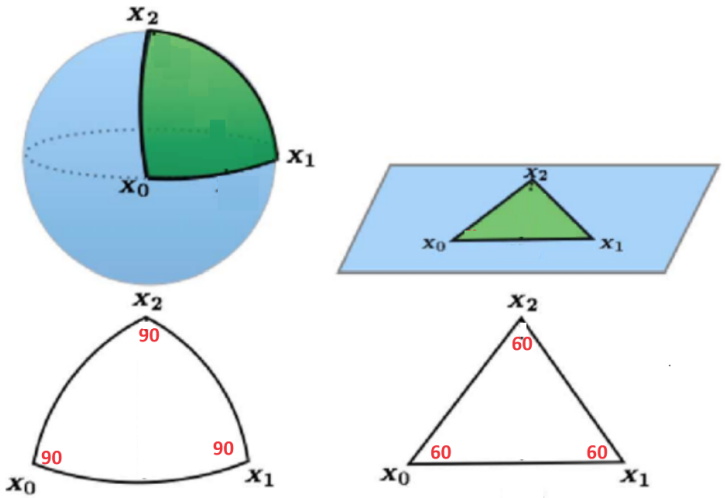
Outline

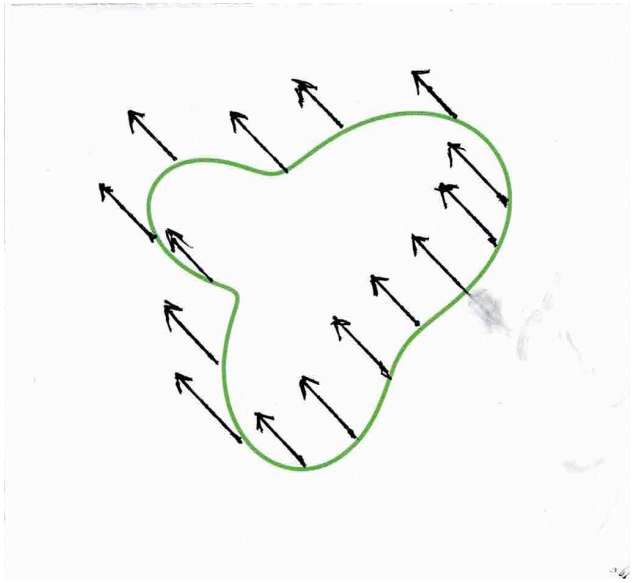
Outline

A simple “curved space”

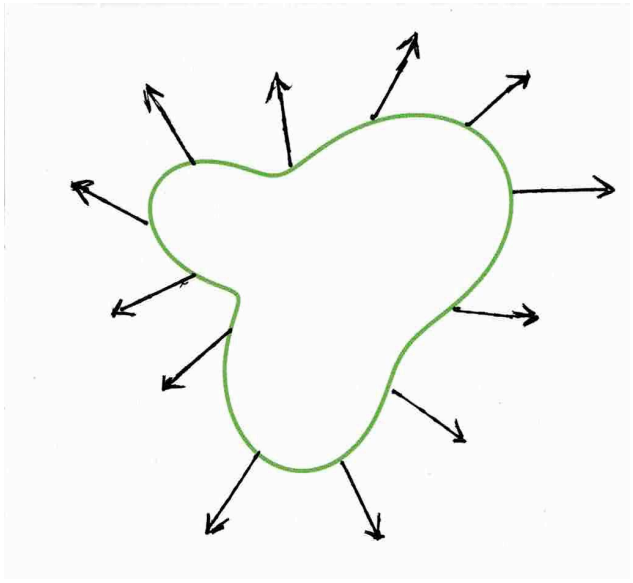


An ant crawling on a 2D surface (space):
How can it discover whether it is flat or curved?

Theorema egregium (Gauss, 1827)



Parallel transport



Arbitrary transport

Theorema egregium: $$\gamma = \oint_{\partial\Sigma} d\phi = \int_{\Sigma} d\sigma\, K \mod 2\pi$$

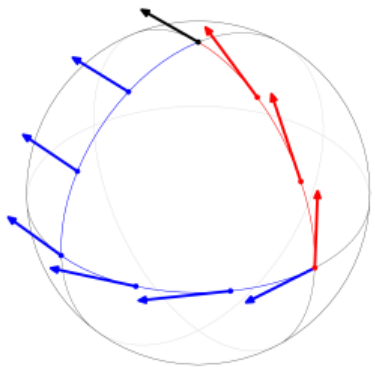
K : Gaussian curvature

Holonomy

Gaussian curvature
of a spherical surface $K = 1/R^2$

Integrated over an octant:

$$\int_\Sigma d\sigma\ K = \frac{1}{8} \times 4\pi R^2 \times \frac{1}{R^2} = \frac{\pi}{2}$$



- Holonomy: Angular mismatch for parallel transport:

$$\gamma = \int_\Sigma d\sigma\ K \qquad \mod 2\pi$$

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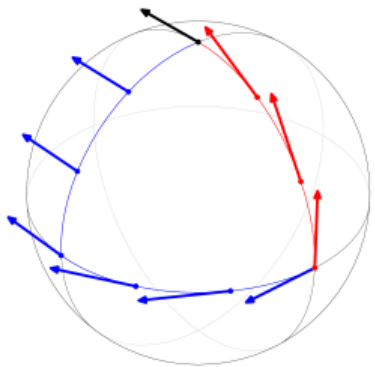

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Berry curvature

- (κ, λ) are the real coordinates of a 2D space
- The time-independent Hamiltonian depends on (κ, λ)
- $|\Psi_n\rangle$ and E_n also depend on (κ, λ)

- **Definition**:

$$\begin{aligned} \Omega(\kappa, \lambda) &= i\left(\langle \partial_\kappa \Psi_0 | \partial_\lambda \Psi_0 \rangle - \langle \partial_\lambda \Psi_0 | \partial_\kappa \Psi_0 \rangle\right) \\ &= -2\,\mathrm{Im}\,\langle \partial_\kappa \Psi_0 | \partial_\lambda \Psi_0 \rangle \end{aligned}$$

- Introduced in the 1980s independently by M. Berry and by D. Thouless & coworkers

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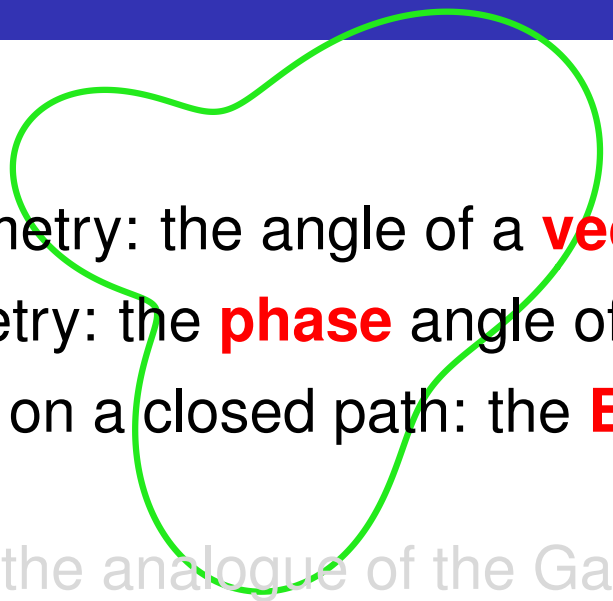


Holonomy:

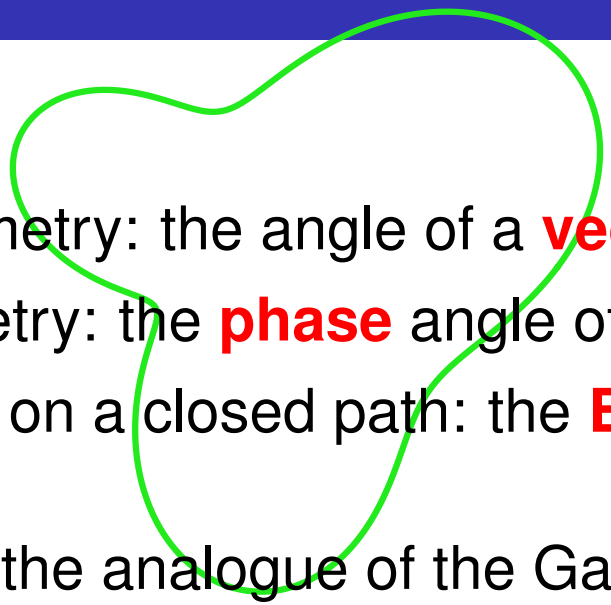
- In differential geometry: the angle of a **vector**
- In quantum geometry: the **phase** angle of a **state vector**
- Angular mismatch on a closed path: the **Berry phase** γ

The Berry curvature is the analogue of the Gaussian curvature

- In differential geometry $\gamma = \oint_{\partial\Sigma} d\phi = \int_{\Sigma} d\sigma \; K$
- In quantum geometry $\gamma = \oint_{\partial\Sigma} d\phi = \int_{\Sigma} d\kappa d\lambda \; \Omega(\kappa, \lambda)$
- Σ domain included by the closed path $\partial\Sigma$

Berry curvature = Berry phase per unit area

Berry phase



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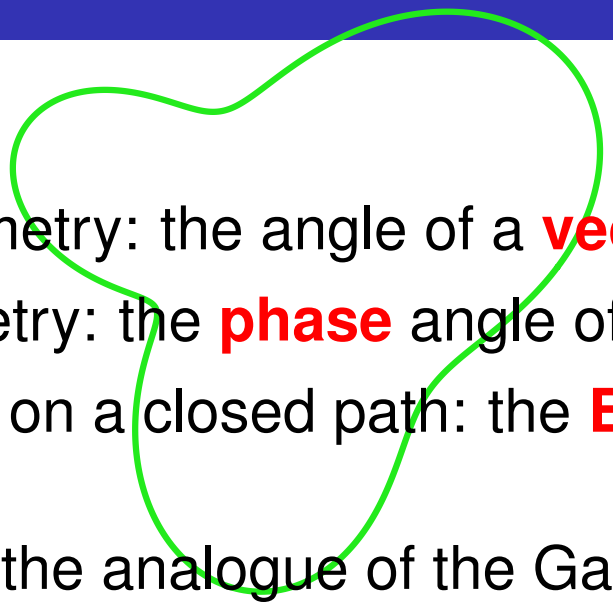

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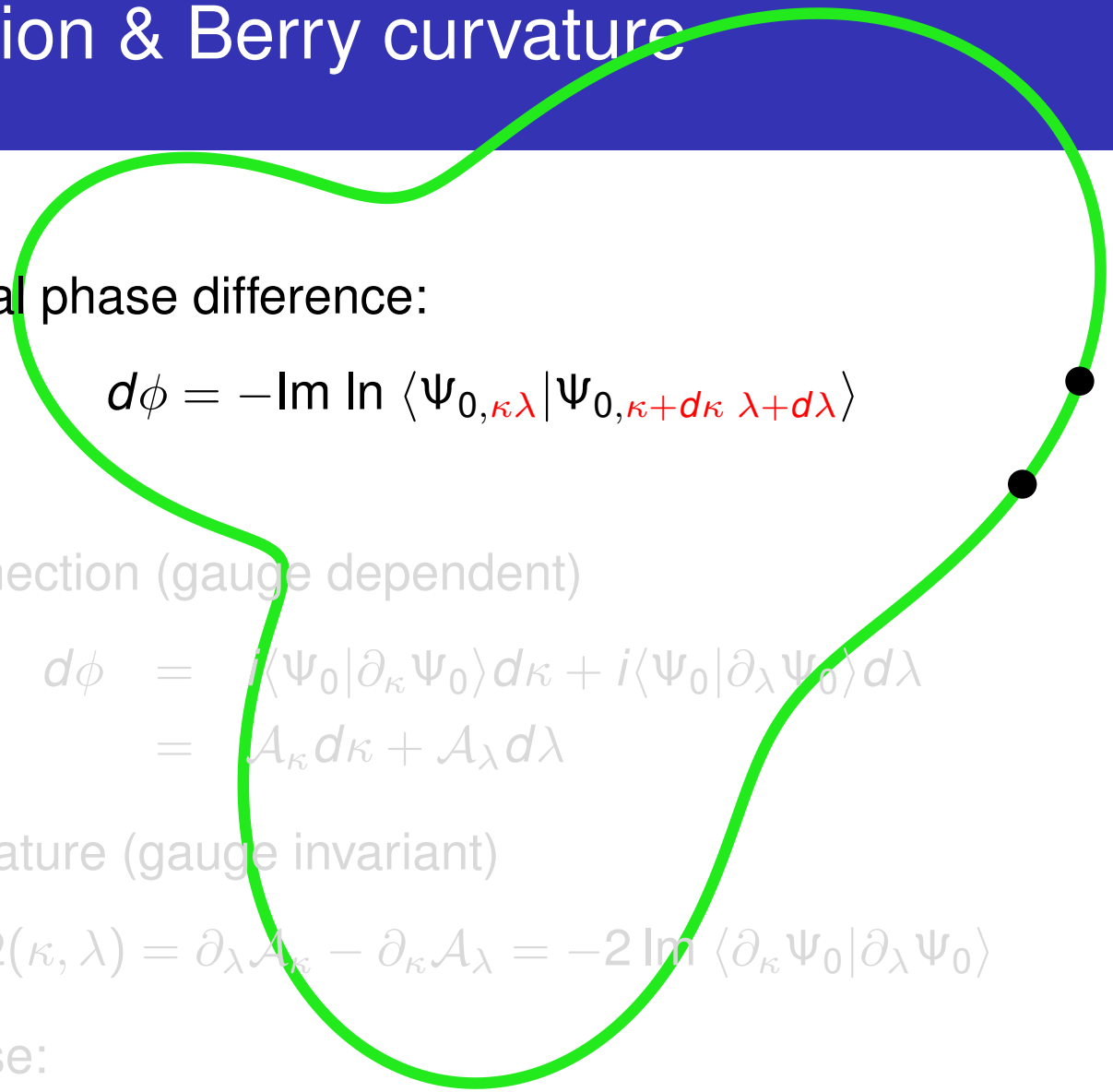
Berry connection & Berry curvature



- Infinitesimal phase difference:

$$d\phi = -\mathrm{Im}\ \ln \langle \Psi_{0,\kappa\lambda} | \Psi_{0,\kappa+d\kappa\ \lambda+d\lambda} \rangle$$

- Berry connection (gauge dependent)

$$\begin{aligned} d\phi &= i\langle \Psi_0 | \partial_\kappa \Psi_0 \rangle d\kappa + i\langle \Psi_0 | \partial_\lambda \Psi_0 \rangle d\lambda \\ &= \mathcal{A}_\kappa d\kappa + \mathcal{A}_\lambda d\lambda \end{aligned}$$

- Berry curvature (gauge invariant)

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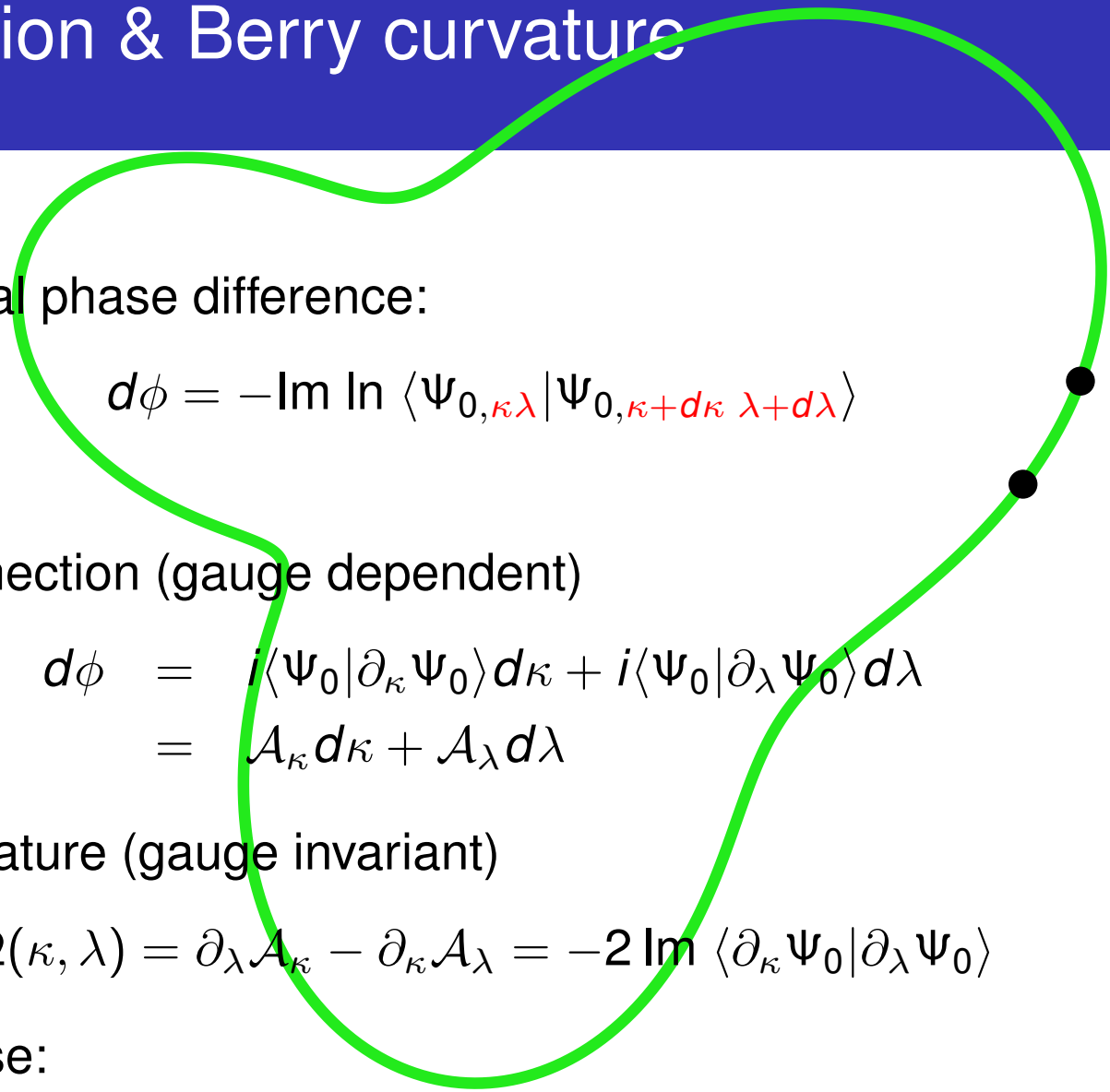

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Alternative expressions

- Berry curvature:

$$\begin{aligned}\Omega(\kappa,\lambda) &= i(\langle\partial_\kappa\Psi_0|\partial_\lambda\Psi_0\rangle - \langle\partial_\lambda\Psi_0|\partial_\kappa\Psi_0\rangle)\\ &= -2\,\mathrm{Im}\,\langle\partial_\kappa\Psi_0|\partial_\lambda\Psi_0\rangle;\end{aligned}$$

- Also expressed as a Kubo formula:

$$\Omega(\kappa,\lambda) = -2\,\mathrm{Im}\sum_{n\neq 0}\frac{\langle\Psi_0|\partial_\kappa\hat{H}|\Psi_n\rangle\langle\Psi_n|\partial_\lambda\hat{H}|\Psi_0\rangle}{(E_0-E_n)^2}.$$

- Also expressed as a trace:

$$\Omega(\kappa,\lambda) = i\,\mathrm{Tr}\,\{\hat{P}\,[\,\partial_\kappa\hat{P},\partial_\lambda\hat{P}\,]\},\qquad \hat{P} = |\Psi_0\rangle\langle\Psi_0|$$

Outline

Time-dependent Hellmann-Feynman

- The time-independent operator $\hat{O}$ can be written as an **Hamiltonian derivative**: $\hat{O} = \partial_\kappa \hat{H}$
- For time-independent λ: Hellmann-Feynman

$$O \equiv \langle \Psi_0 | \hat{O} | \Psi_0 \rangle = \partial_\kappa E_0$$

- When $\lambda \to \lambda(t)$, then $\hat{H} \to \hat{H}_t$, $E(t) = \langle \Psi_t | \hat{H}_t | \Psi_t \rangle$

$$\begin{aligned} \partial_\kappa E(t) &= \langle \Psi_t | \hat{O} | \Psi_t \rangle + \langle \partial_\kappa \Psi_t | \hat{H}_t | \Psi_t \rangle + \langle \Psi_t | \hat{H}_t | \partial_\kappa \Psi_t \rangle \\ &= O(t) + i\hbar(\langle \partial_\kappa \Psi | \dot{\Psi}_t \rangle - \langle \dot{\Psi} | \partial \kappa \Psi_t \rangle) \end{aligned} \tag{1}$$

- **Exact** time-evolution of $\langle \hat{O}(t) \rangle$:

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- **Kato's theorem (1950):**
  "when the change of the Hamiltonian in time is made infinitely slow, the system, when started from a stationary state, passes through the corresponding stationary states for all times".

- All quantities replaced with their instantaneous value at $\lambda = \lambda(t)$

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nongeometric **geometric**

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Beyond Hellmann-Feynman

- When $\hat{O} = \partial_\kappa \hat{H}$:

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- When $\hat{O}$ **cannot** be written as an Hamiltonian derivative

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- Both expressions exact in the **adiabatic limit**:
  - They differ from the exact evolution by terms of order $\ddot{\lambda}$
  - If the evolution is harmonic, they are exact to order ω and neglect terms of order ω^2

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- When the system is time-reversal invariant
  - Hamiltonian & eigenfunctions real
  - For a **real** $\hat{O}$: Only the first term is nonvanishing (like e.g. the electron density)
  - For an **imaginary** $\hat{O}$: Only the second term is nonvanishing (like e.g. the current density)
  - For an **imaginary** $\hat{O} = \partial_\kappa \hat{H}$:

$$\frac{O(t)}{\dot{\lambda}(t)} = -\hbar \Omega(\kappa, \lambda) \qquad \text{(Adiabatic Hellmann-Feynman)}$$

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Kohn's (1964) Hamiltonian

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m} \sum_{i=1}^{N} [\mathbf{p}_i + \hbar\boldsymbol{\kappa}]^2 + \hat{V}$$

- Macroscopically homogeneous system
- N electrons in a cubic box **(supercell)** of volume L^d
- $\hat{V}$ one-body and two-body potentials
- Time-reversal invariant af $\kappa = 0$
- Born-von-Kàrmàn PBCs:
  The coordinates $r_{i\alpha}$ are actually **angles** $\varphi_{i\alpha} = 2\pi r_{i\alpha}/L$

- κ-derivatives taken **first**, $L \to \infty$ limit **after**:
  This warrants adiabaticity even in metals
  CAVEAT: DFT implicitly takes the limit in a different order!

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The $\boldsymbol{\kappa}$ parameter

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m}\sum_{i=1}^{N}[\mathbf{p}_i + \hbar\boldsymbol{\kappa}]^2 + \hat{V}$$

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

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

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

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

Adiabatic current density (many-body formula)

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m}\sum_{i=1}^{N}(\mathbf{p}_i + \hbar\boldsymbol{\kappa})^2 + \hat{V}_\lambda$$

- Macroscopic current-density operator:

$$\hat{j}_\alpha = -\frac{e}{L^d}\hat{v}_\alpha = -\frac{e}{mL^d}\sum_{i=1}^{N} p_{i\alpha} = -\frac{e}{\hbar L^d}\partial_{\kappa_\alpha}\hat{H}_{\boldsymbol{\kappa}}$$

- Adiabatic Hellmann-Feynman:

$$j_\alpha(t) = -\frac{e}{\hbar L^d}\left[\partial_{\kappa_\alpha} E_0 - \hbar\,\Omega(\kappa_\alpha,\lambda)\dot{\lambda}(t)\right]$$

nongeometric **geometric**

Kohn-Sham Hamiltonian (in crystals)

- Kohn-Sham energies & periodic Bloch orbitals:

$$\epsilon_{j\mathbf{k}}, \qquad |\psi_{j\mathbf{k}}\rangle = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}|u_{j\mathbf{k}}\rangle$$

- Kohn-Sham Hamiltonian with a "flux":

$$\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}} H_{\boldsymbol{\kappa}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{2m}\left[\mathbf{p} + \frac{e}{c}\mathbf{A}(\mathbf{r}) + \hbar\mathbf{k} + \hbar\boldsymbol{\kappa}\right]^2 + V_{\mathrm{KS}}(\mathbf{r}),$$

- **Conversion recipe** Many-body $\longrightarrow$ Kohn-Sham:
  1. Make the quantity intensive (when needed)
  2. Replace $\boldsymbol{\kappa}$-derivatives with $\mathbf{k}$-derivatives
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Outline

Definition

- Key entries for infrared absorption in **insulating** solids & for charge transport in liquid electrolytes

- $Z^*_{s,\alpha\beta}$ = derivative of the macroscopic polarization **P** wrt nuclear displacement of nucleus s

$$Z^*_{s,\alpha\beta} = \frac{L^d}{e}\frac{\partial P_\alpha}{\partial R_{s,\beta}}$$

- Nuclei adiabatically displaced in time:

$$Z^*_{s,\alpha\beta} = \frac{L^d}{e}\frac{\partial P_\alpha/\partial t}{\partial R_{s,\beta}/\partial t} = Z_s\delta_{\alpha\beta} + \frac{L^d}{e}\frac{j_\alpha(t)}{\dot{R}_{s,\beta}}$$

Berry-curvature formula

- Adiabatic Hellmann-Feynman:

$$Z^*_{s,\alpha\beta} = Z_s\delta_{\alpha\beta} + \frac{L^d}{e}\frac{j_\alpha(t)}{\dot{R}_{s,\beta}}$$

$$\text{Many-body} \quad = Z_s\delta_{\alpha\beta} + \Omega(\kappa_\alpha, R_{s,\beta})\Big|_{\boldsymbol{\kappa}=0,\,\mathbf{R}_s}$$

$$\text{Kohn-Sham} \quad = Z_s\delta_{\alpha\beta} + V_{\text{cell}}\sum_j \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^d} f_j(\mathbf{k})\,\tilde{\Omega}_j(k_\alpha, R_{s,\beta})$$

- Single-particle Berry curvature of band j:
(King-Smith & Vanderbilt, 1993)

$$\tilde{\Omega}_j(k_\alpha, R_{s,\beta}) = -2\,\text{Im}\,\langle\partial_{k_\alpha} u_{j\mathbf{k}}|\partial_{R_{s\beta}} u_{j\mathbf{k}}\rangle$$

Acoustic sum rule

- Born charge as a single-point Berry curvature:

$$Z^*_{s,\alpha\beta} = Z_s \delta_{\alpha\beta} + \Omega(\kappa_\alpha, R_{s,\beta})$$

- Holds as it stands for insulators **and metals**
  - where **P** does not makes sense
  - where the $Z^*_{s,\alpha\beta}$ are unrelated to infrared absorption

- A rigid translation of the lattice: $\mathbf{R}_s(t) = \mathbf{u}(t)$, any s

$$j_\alpha(t) = \left(\sum_s Z^*_{s,\alpha\beta} \right) \dot{u}_{\beta,s}$$

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- Do the **exact** and **Kohn-Sham** $Z^*_{s,\alpha\beta}$ coincide?
  - **YES** in molecules
  - **NO** in solids!

- **Why?**
  - The famous G^3 (Gonze-Ghosez-Godby) 1995 paper
  - Is the discrepancy a serious drawback?

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  - So-called adiabatic TDDFT does **not** access adiabatic response properties!
  - One needs nonadiabatic TDDFT or (even better) TDCDFT !

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Outline

Free acceleration in metals

- Classical Drude theory (A.D. 1900), dissipationless limit

$$\mathbf{j}(t) = e^2 \frac{n}{m} \mathcal{E} t$$

- $n = N/L^d$ conduction-electron density
- n/m **inverse inertia of the many-electron system**

- Fourier transform (singular):

$$\mathbf{j}(\omega) = \sigma^{(\mathrm{Drude})}(\omega) \mathcal{E}(\omega)$$

- Enforcing causality (Ashcroft-Mermin, Ch. 1):

$$\sigma^{(\mathrm{Drude})}(\omega) = D \left[\delta(\omega) + \frac{i}{\pi \omega} \right], \qquad D = \frac{\pi e^2 n}{m}$$

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Electronic current induced by a dc field

- Adiabatic Hellmann-Feynman once more:

$$j_\alpha(t) = -\frac{e}{\hbar L^d}\left[\partial_{\kappa_\alpha} E_0 - \hbar\,\Omega(\kappa_\alpha, \lambda)\dot{\lambda}(t)\right]$$

- Identify $\lambda(t) \longrightarrow \kappa_\beta(t) = -\frac{e}{\hbar}\mathcal{E}_\beta\, t$
- Longitudinal & transverse currents:

$$j_\alpha(t) = -\frac{e}{\hbar L^d}\partial_{\kappa_\alpha} E_0 + \frac{e^2}{L^d}\Omega(\kappa_\alpha, \kappa_\beta)\mathcal{E}_\beta$$

- $\Omega(\kappa_\alpha, \kappa_\beta) = 0$ in a T-invariant system

Longitudinal response

- In a dc field the electrons undergo free acceleration:

$$\partial_t j_\alpha(t) = e^2 \frac{n^*_{\alpha\beta}}{m} \mathcal{E}_\beta$$

- Longitudinal current

$$\begin{aligned} j_\alpha(t) &= -\frac{e}{\hbar L^d} \partial_{\kappa_\alpha} E_0 \\ \partial_t j_\alpha(t) &= -\frac{e}{\hbar L^d} \frac{\partial^2 E_0}{\partial \kappa_\alpha \partial t} = -\frac{e}{\hbar L^d} \frac{\partial^2 E_0}{\partial_{\kappa_\alpha} \partial_{\kappa_\beta}} \dot{\kappa}_\beta = \frac{e^2}{\hbar^2 L^d} \frac{\partial^2 E_0}{\partial_{\kappa_\alpha} \partial_{\kappa_\beta}} \mathcal{E}_\beta \end{aligned}$$

- Inverse inertia:

$$\frac{n^*_{\alpha\beta}}{m} = \frac{1}{\hbar^2 L^d} \frac{\partial^2 E_0}{\partial_{\kappa_\alpha} \partial_{\kappa_\beta}}$$

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Drude weight (a.k.a. adiabatic charge stiffness)

- Fourier transform:

$$j_\alpha(t) = \frac{e^2}{\hbar^2 L^d} \frac{\partial^2 E_0}{\partial_{\kappa_\alpha} \partial_{\kappa_\beta}} \mathcal{E}_\beta t \qquad j_\alpha(\omega) = \sigma^{(\mathrm{Drude})}_{\alpha\beta}(\omega) \mathcal{E}_\beta(\omega)$$

- Enforcing causality:

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

- The famous Kohn's formula (1964):

$$D_{\alpha\beta} = \frac{\pi e^2}{m} n^*_{\alpha\beta} = \frac{\pi e^2}{\hbar^2 L^d} \frac{\partial^2 E_0}{\partial_{\kappa_\alpha} \partial_{\kappa_\beta}}$$

Kohn-Sham optical conductivity

$$j_\alpha(\omega) = \sigma_{\alpha\beta}(\omega) E_\beta(\omega), \qquad \sigma_{\alpha\beta}(\omega) = \sigma^{(+)}_{\alpha\beta}(\omega) + \sigma^{(-)}_{\alpha\beta}(\omega)$$

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

- Adiabatic TDDFT:
  - Filled bands don't contribute. Kohn's formula yields:

$$D_{\alpha\beta} = \frac{2\pi e^2}{\hbar^2} \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^3} f(\epsilon_\text{F} - \epsilon_\mathbf{k}) \frac{\partial^2 \epsilon_\mathbf{k}}{\partial k_\alpha \partial k_\beta}$$

  - $\sigma^{(\text{regular})}_{\alpha\beta}(\omega)$ is nonadiabatic: interband Kubo formula

Fermi-volume & Fermi-surface formulæ for $D_{\alpha\beta}$

- Integrating by parts

$$\begin{aligned} D_{\alpha\beta} &= \frac{2\pi e^2}{\hbar^2} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^3} f(\epsilon_{\mathrm{F}} - \epsilon_{\mathbf{k}}) \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_\alpha \partial k_\beta} \\ &= -\frac{2\pi e^2}{\hbar^2} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^3} f'(\epsilon_{\mathbf{k}}) \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\alpha} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\beta} \end{aligned} \tag{2}$$

- Velocity of a band electron

$$v_{\mathbf{k},\alpha} = \frac{1}{\hbar} \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\alpha} \quad \rightarrow \quad D_{\alpha\beta} = -2\pi e^2 \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^3} f'(\epsilon_{\mathbf{k}})\, v_{\mathbf{k},\alpha} v_{\mathbf{k},\beta}$$

- In agreement with **Landau's Fermi-liquid theory**: Intraband quasiparticle property

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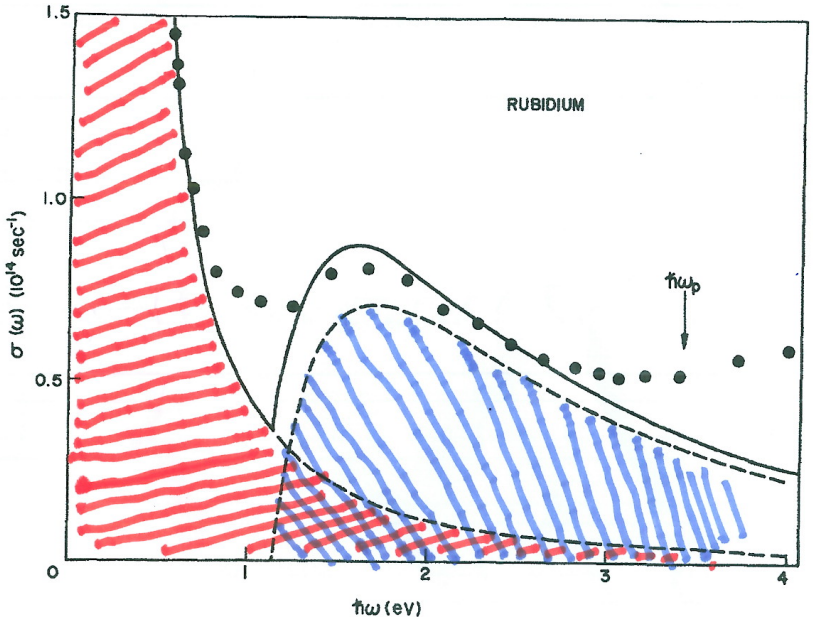
Experiment: Drude term & regular term

- $\sigma_{\alpha\beta}^{(\mathrm{Drude})}(\omega)$ **Intra**band from Kohn's adiabatic formula
  Main issue:
  Is it broadened by **extrinsic** or **intrinsic** effects?
- $\sigma_{\alpha\beta}^{(\mathrm{regular})}(\omega)$ **Inter**band from Kubo formula

$\sigma(\omega)$ in Rubidium

- **Dots:** experiment
- **Red:** Drude
- **Blue:** Regular
- **Solid:** sum of the two terms



Drude peak broadening: Extrinsic vs. intrinsic

- Kohn's prescription:
  - κ-derivatives taken **first**, $L \to \infty$ limit **after**
  - Response causal but **nondissipative** at any L

$$\sigma_{\alpha\beta}^{(\mathrm{Drude})}(\omega) = \lim_{\eta \to 0^+} \frac{D_{\alpha\beta}}{\pi} \frac{i}{\omega + i\eta} = D_{\alpha\beta} \left[\delta(\omega) + \frac{i}{\pi\omega} \right]$$

- DFT: *Theory of the Inhomogeneous Electron Gas*
  - $L \to \infty$ limit **first**: **k** becomes a continuous variable
  - The crystalline potential is switched on afterwards
  - Memory-dependent functionals:
    The dc response becomes nonadiabatic & **dissipative**

- Dissipation (a.k.a. Joule heating) with no relaxation time:
  - Giuliani-Vignale:
    An infinite system is its own thermostat

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Dreyer-Coh-Stengel sum rule (2022)

- Acoustic sum rule (Pick, Cohen, & Martin 1970):

$$\sum_s Z^*_{s,\alpha\beta} = 0 \qquad \textbf{in insulators only}$$

- In metals the electrons are left behind, $\mathbf{j}(t) \neq 0$
- In the reference frame of the nuclei the current is carried by the electrons, all moving with velocity $-\dot{\mathbf{u}}$:

$$j_\alpha(t) = e\, n^*_{\alpha\beta} \dot{u}_\beta = \frac{e}{L^d} \left(\sum_s Z^*_{s,\alpha\beta} \right) \dot{u}_\beta$$

- **Outstanding message:**

  A macroscopic $\mathcal{E}$ field and a rigid translation of the lattice probe the same material property: $n^*_{\alpha\beta}$

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- **Outstanding message:**

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Outline

Breaking time-reversal symmetry

- Modified Hamiltonian: $\mathbf{A}^{(\mathrm{micro})}(\mathbf{r})$ **intrinsic** T-breaking term

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

- The adiabatic current, again:

$$j_\alpha(t) = -\frac{e}{\hbar L^d}\partial_{\kappa_\alpha} E_0 + \frac{e^2}{L^d}\Omega(\kappa_\alpha, \kappa_\beta)\mathcal{E}_\beta$$

- Anomalous Hall conductivity (**intrinsic**, or geometric):

$$j_\alpha^{(\mathrm{Hall})} = \sigma_{\alpha\beta}^{(-)}\mathcal{E}_\beta \qquad \longrightarrow \qquad \sigma_{\alpha\beta}^{(-)} = \frac{e^2}{L^d}\Omega(\kappa_\alpha, \kappa_\beta)$$

AHC as a single-point Berry curvature

$$\sigma^{(-)}_{\alpha\beta} = -\frac{e^2}{\hbar L^d}\Omega(\kappa_\alpha, \kappa_\beta)$$

- Curvature evaluated at $\boldsymbol{\kappa} = 0$
- Very general: 2d and 3d, metals and insulators
- Topological for a **2d insulator**
- Extrinsic effects:
  - Very relevant in metals
  - Nonexisting in the topological case
  - For noninteracting electrons (Kohn-Sham) it coincides with the standard Fermi-volume integral in the $L \to \infty$ limit

QAHE (quantum anomalous Hall effect)

$$\sigma_{xy}^{(-)} = -\frac{e^2}{\hbar} \times \frac{1}{L^2}\Omega(\kappa_x, \kappa_y)\Big|_{\boldsymbol{\kappa}=0}$$

,

- **A universal constant $\times$ a dimensionless quantity**
- Quantized in the **insulating** case
- Topological quantization for $L \to \infty$, **not** for finite L

$$\frac{h}{e^2}\sigma_{xy}^{(-)} = \lim_{L\to\infty} \frac{2\pi}{L^2}\Omega(\kappa_x, \kappa_y)\Big|_{\boldsymbol{\kappa}=0} = \quad C_1 \in \mathbb{Z}$$

- Natural resistance unit:
  1 klitzing $= h/e^2 = 25812.807557(18)$ ohm

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An early simulation

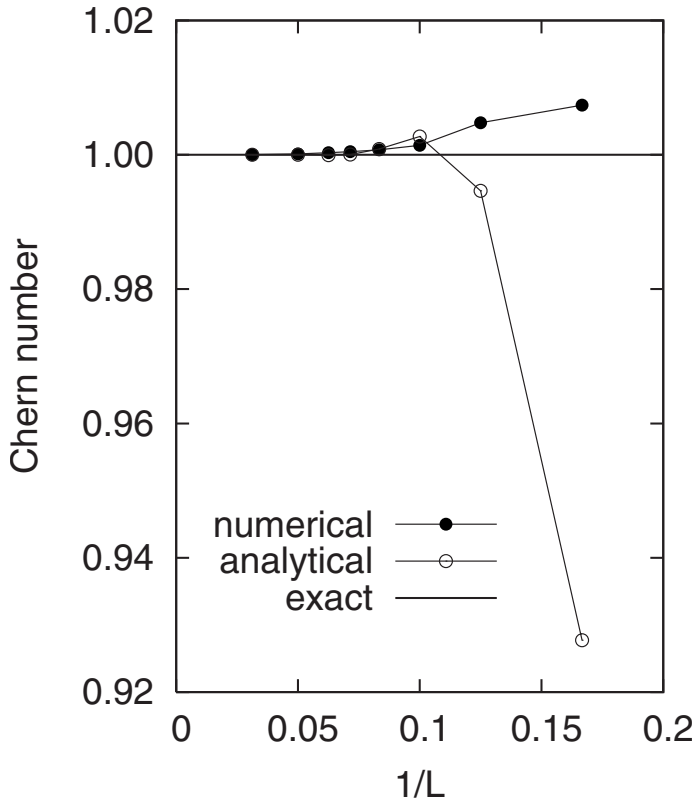
D. Ceresoli & R. Resta, Phys. Rev. B **76**, 012405 (2007)

Single-point Berry curvature

Haldane (noninteracting) model Hamiltonian

Convergence:

$$\frac{2\pi}{L^2}\Omega(\kappa_x,\kappa_y)\Big|_{\boldsymbol{\kappa}=0} \rightarrow C_1$$

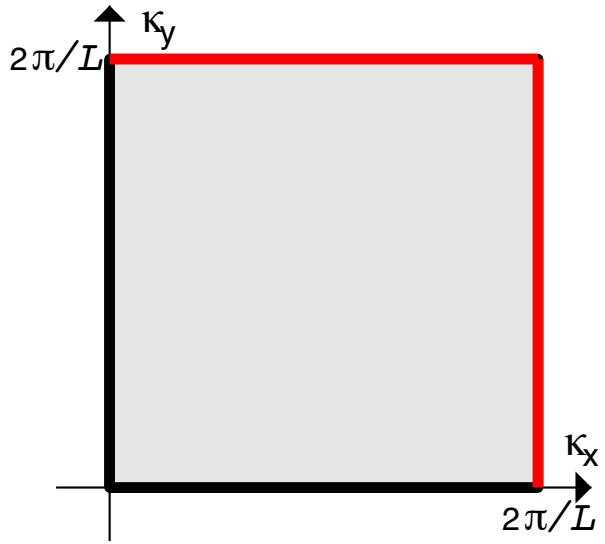


Many-body Chern number

Q. Niu, D. J. Thouless, and Y. S. Wu, Phys. Rev. B **31**, 3372 (1985)

The mean-value theorem:

$$\frac{4\pi^2}{L^2}\Omega(\kappa_x,\kappa_y)\Big|_{\boldsymbol{\kappa}=0} \simeq \int_0^{\frac{2\pi}{L}} d\kappa_x \int_0^{\frac{2\pi}{L}} d\kappa_y\, \Omega(\kappa_x,\kappa_y)$$



Integral over a torus in the **insulating case only**
Quantized for any L

$$\frac{2\pi}{L^2}\Omega(\kappa_x,\kappa_y)\Big|_{\boldsymbol{\kappa}=0} \simeq \frac{1}{2\pi}\int_0^{\frac{2\pi}{L}} d\kappa_x \int_0^{\frac{2\pi}{L}} d\kappa_y\, \Omega(\kappa_x,\kappa_y) = C_1$$

Outline

Outlook

- The Berry curvature:
  - The main entity addressing adiabatic quantum transport
  - Independently introduced
    by Berry and by Thouless in the 1980s
- Geometrical observables (in this talk):
  - Born effective charges, dc conductivity
    (longitudinal & transverse)
  - Here: compact many-body formulæ
    (conversion into KS formulæ is straightforward)
- A subtle issue:
  Adiabatic in many-body setting vs. DFT-adiabatic

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