

↓ Lecture 5 [25.04.25]

iii | \triangleleft Adiabatic theorem

 \rightarrow Initial state remains in the ground state manifold: $|\Psi(t)\rangle \in \mathcal{V}(\Gamma(t)) \rightarrow$

(L) $|\Psi(t)\rangle = \sum_{i=1}^{n} \Psi_i(t) |v_i(\Gamma(t))\rangle \rightarrow$

 $\partial_t |\Psi(t)\rangle = (\partial_t \Psi_i(t)) |v_i(\mathbf{\Gamma}(t))\rangle + \Psi_i(t) [\partial_{\Gamma_l} |v_i(\mathbf{\Gamma}(t))\rangle] (\partial_t \Gamma_l(t)) \quad (1.31)$

We omit sum symbols; sums over repeated indices are implied (Einstein notation).

(R) $H(\Gamma(t))|\Psi(t)\rangle = 0$ (Remember that we set the ground state energy to zero.)

This assumption is not crucial for the derivation that follows; it simply removes any dynamical phase from the evolution, so that only a geometric phase remains (which is what we are interested in). If you do not set the ground state energy to zero, use $H(\Gamma(t))|\Psi(t)\rangle = E_0(\Gamma(t))|\Psi(t)\rangle$ instead and track the additional term. Its effect is to add an additional, energy-dependent dynamical phase to the evolution of the wave function (which is not a new & interesting insight ...).

iv | Apply $\langle v_j(\mathbf{\Gamma}(t)) |$ and use Eq. (1.30):

$$\partial_t \Psi_j(t) = -\Psi_i(t) \left\langle v_j(\boldsymbol{\Gamma}(t)) | \partial_{\Gamma_l} | v_i(\boldsymbol{\Gamma}(t)) \right\rangle \left(\partial_t \Gamma_l(t) \right)$$
(1.32)

v | This suggests the definition of the

** Berry connection
$$[\mathcal{A}_{l}(\Gamma)]_{ji} := -i \langle v_{j}(\Gamma) | \partial_{\Gamma_{l}} | v_{i}(\Gamma) \rangle \in \mathfrak{u}(n)$$
 (1.33)

Think of the A_l as Γ -dependent Hermitian $n \times n$ -matrices, one for each of the l = 1, ..., k parameters.

vi | With this definition, we can write $[\Psi \equiv (\Psi_j)_{j=1,...,n}]$

$$\partial_{t} \Psi(t) = -i \underbrace{(\partial_{t} \Gamma_{l}(t)) \mathcal{A}_{l}(\Gamma(t))}_{\text{Time-dependent matrix}} \Psi(t)$$
(1.34)

vii | This equation can be solved with a \checkmark Time- (T) or path-ordered (P) exponential:

$$\Psi(T) = \mathcal{T} \exp\left[-i \int_0^T \mathcal{A}_l(\Gamma(t)) \,\partial_t \Gamma_l(t) \,\mathrm{d}t\right] \Psi_0 \tag{1.35a}$$

$$= \underbrace{\mathcal{P} \exp\left[-i \int_{\Gamma} \mathcal{A} d\Gamma\right]}_{\equiv U_{\Gamma} \text{ (Unitary matrix)}} \Psi_{0} \tag{1.35b}$$

Here, $\mathbf{A} = (A_l)$ should be seen as a u(n)-valued vector field on the parameter space (a 1-form). I.e., \mathbf{A} can be integrated along parameter paths which, after (path ordered) exponentiation, produces a unitary U(n) that describes the geometric part of the adiabatic evolution on the ground state space.



Note that the choice of basis is a gauge choice: it cannot have physical significance!

$$\stackrel{\circ}{\to} \quad \mathcal{A}_{l}^{\prime} = \Omega \mathcal{A}_{l} \Omega^{\dagger} - i \frac{\partial \Omega}{\partial \Gamma_{l}} \Omega^{\dagger}$$
(1.36)

If you attended a course on quantum field theory, you might recognize this as the gauge transformation of a non-abelian U(n)/SU(n) Yang-Mills gauge theory (like QCD). The difference is that here the gauge (Berry) connection A_l does not live on Minkowski spacetime but on an abstract "parameter space." Gauge transformations arise from "parameter-local" basis transformations in the degenerate ground state space of a Hamiltonian (family).

$$\stackrel{\circ}{\to} \quad U_{\Gamma}' = \Omega(\Gamma(T)) \, U_{\Gamma} \, \Omega^{\dagger}(\Gamma(0)) \tag{1.37}$$

To show this, consider an infinitesimal piece d Γ of the path Γ and linearize U_{Γ} along this piece to derive the above transformation. Then use that the path-ordered exponential is defined as the product of such infinitesimal pieces. The identity $\Omega \frac{\partial \Omega^{\dagger}}{\partial \Gamma_{L}} = -\frac{\partial \Omega}{\partial \Gamma_{L}} \Omega^{\dagger}$ might help (prove this!).

6 $| \triangleleft \text{Open path } \Gamma \rightarrow U_{\Gamma} \text{ is gauge dependent } \rightarrow \text{Cannot contain physical information!}$

To see this let $\Omega(\Gamma(0)) = \mathbb{1}$. Then $U'_{\Gamma} = \Omega(\Gamma(T)) U_{\Gamma}$ can be chosen (almost) *arbitrary* since U(n) is a group and $\Omega(\Gamma(T))$ can be chosen (almost) arbitrary (just connect it smoothly to the identity, i.e., its determinant must be one). This means that U_{Γ} cannot contain physical information as it can be transformed into any other unitary U'_{Γ} (with the same determinant) by parameter-local basis transformations.

 $\rightarrow \triangleleft \underline{\text{Closed}} \text{ loops } \Gamma \text{ in parameter space}$

I.e., $H(\Gamma(0)) = H(\Gamma(T))$ and $\mathcal{V}(\Gamma(0)) = \mathcal{V}(\Gamma(T))$ such that U_{Γ} is an *automorphism* on $\mathcal{V}(\Gamma(0))$ and described the geometric transformation of ground states due to cyclic (and adiabatic) deformations of the Hamiltonian.

 $\mathbf{7}$ | Then the

** Berry holonomy
$$U_{\Gamma} = \mathcal{P} \exp\left[-i \oint_{\Gamma} \mathcal{A} d\Gamma\right] \in \mathrm{U}(n)$$
 (1.38)

is gauge covariant: [This follows from the continuity of $\Omega(\Gamma)$ and $\Gamma(T) = \Gamma(0)$.]

$$U_{\Gamma}' = \Omega(\Gamma(0)) U_{\Gamma} \Omega^{\dagger}(\Gamma(0))$$
(1.39)

Note that the argument from above breaks down since both unitaries $\Omega(\Gamma(T)) = \Omega(\Gamma(0))$ are necessarily the same (since the parameter path is closed). U_{Γ} can still be changed, but not arbitrarily: It is unique up to unitary basis transformations (for instance, its spectrum is independent of basis changes!). This quantity *can* encode physical properties of the system. Note the difference between gauge *invariant* $(U'_{\Gamma} = U_{\Gamma})$ and gauge *covariant* [Eq. (1.39)].

8 | There is another important *gauge covariant* quantity (that we will use \rightarrow *below*):

** Berry curvature
$$\mathcal{F}_{lm} := \frac{\partial \mathcal{A}_l}{\partial \Gamma_m} - \frac{\partial \mathcal{A}_m}{\partial \Gamma_l} - i \left[\mathcal{A}_l, \mathcal{A}_m\right] \in \mathfrak{u}(n)$$
 (1.40)

oreti



This is the "field-strength" of the gauge field \mathcal{A} , the non-abelian generalization of the field-strength tensor $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$ in electrodynamics (where $A_{\mu} \in \mathfrak{u}(1) \simeq \mathbb{R}$ so that the commutator vanishes identically).

 $\rightarrow \mathcal{F}_{lm}$ is gauge covariant:

$$\mathcal{F}'_{ij}(\Gamma) \stackrel{\circ}{=} \Omega(\Gamma) \,\mathcal{F}_{ij}(\Gamma) \,\Omega^{\dagger}(\Gamma) \tag{1.41}$$

Notes:

- This is the field strength tensor known from ↑ non-abelian Yang-Mills gauge theories. The Yang-Mills Lagrangian takes the trace of the field strength tensor, thereby converting a gauge covariant quantity into a gauge invariant quantity: Tr[F_{μν} F^{μν}]. (Note that the summation over μ and ν is not related to gauge but Lorentz invariance for YM theories; as we do not have generic symmetries on the parameter space, we do not have an analog of this symmetry in the current situation.)
- If Eq. (1.40) seems abstract but you know about ↓ general relativity, there is some insightful connection (☉) to be drawn. Remember that the ↓ Riemann curvature tensor can be expressed as [68, Section 10.2.3]

$$R^{i}{}_{jlm} = \partial_l \Gamma^{i}{}_{jm} - \partial_m \Gamma^{i}{}_{jl} + \Gamma^{i}{}_{nl} \Gamma^{n}{}_{jm} - \Gamma^{i}{}_{nm} \Gamma^{n}{}_{jl}$$
(1.42)

in terms of \checkmark *Christoffel symbols* Γ^{i}_{jm} , which are the (coordinate-dependent) connection coefficients of the (metric-induced) \checkmark *Levi-Civita connection* on the spacetime manifold. Let us interpret the first two indices of the Christoffel symbols as indices of a $D \times D$ matrix (where D is the spacetime dimension), $[\Gamma_{m}]_{ij} \equiv \Gamma^{i}_{jm}$, and do the same for the Riemann curvature tensor: $[R_{lm}]_{ij} \equiv R^{i}_{\ \ \ lm}$. In this notation, Eq. (1.42) reads

$$\boldsymbol{R}_{lm} = \partial_l \boldsymbol{\Gamma}_m - \partial_m \boldsymbol{\Gamma}_l + \boldsymbol{\Gamma}_l \boldsymbol{\Gamma}_m - \boldsymbol{\Gamma}_m \boldsymbol{\Gamma}_l = \partial_l \boldsymbol{\Gamma}_m - \partial_m \boldsymbol{\Gamma}_l - [\boldsymbol{\Gamma}_m, \boldsymbol{\Gamma}_l]$$
(1.43)

which is (up to prefactors) completely analogous to Eq. (1.40). This explains why the Berry curvature is called "curvature": it describes a generalized (and rather abstract) curvature of the vector bundle defined by the ground state spaces $\mathcal{V}(\Gamma)$ on the parameter manifold \mathcal{M} .

Note that in general relativity, the vector space at each point of the spacetime manifold is given by the \checkmark *tangent space* – which has the same dimension as the manifold itself. This is why it is covenient to treat all four indices of the Riemann tensor on the same footing. In our context, the parameter manifold is *k*-dimensional and has nothing to do with the attached ground state spaces $\mathcal{V}(\Gamma)$ that are *n*-dimensional. Hence we prefer the matrix notation in Eq. (1.40) where the indices that correspond to the Hilbert space are suppressed.

1.3.1. Berry phase and Chern number

We now want to focus on the important special case w/o degeneracy (n = 1). In this case, we can make use of the Berry curvature to calculate the Berry holonomy (which is for n = 1 just a phase known as \rightarrow Berry phase):

9 $| \triangleleft$ Special case n = 1: $\mathcal{V}(\Gamma) = \text{span} \{ |v(\Gamma) \rangle \}$ (= systems w/o ground state degeneracy) In this special case, the quantities introduced above simplify as follows:

Berry connection:
$$\mathcal{A}_{l}(\mathbf{\Gamma}) = -i \langle v(\mathbf{\Gamma}) | \partial_{\mathbf{\Gamma}_{l}} | v(\mathbf{\Gamma}) \rangle \in \mathfrak{u}(1) \simeq \mathbb{R}$$
 (1.44a)

Berry holonomy:
$$U_{\Gamma} = \exp\left[-i\oint_{\Gamma} \mathcal{A}d\Gamma\right] \equiv e^{i\gamma(\Gamma)} \in \mathrm{U}(1)$$
 (1.44b)

Berry curvature:
$$\mathcal{F}_{lm} = \frac{\partial \mathcal{A}_l}{\partial \Gamma_m} - \frac{\partial \mathcal{A}_m}{\partial \Gamma_l} \in \mathfrak{u}(1) \simeq \mathbb{R}$$
 (1.44c)



 \rightarrow Ground state can only change by a phase!

10 | Gauge transformation: $\Omega(\Gamma) = e^{i\xi(\Gamma)} \rightarrow$

The gauge transformation of the Berry connection is similar to electrodynamics:

$$\mathcal{A}' = \mathcal{A} + \nabla_{\Gamma} \xi \tag{1.45a}$$

$$U'_{\Gamma} = U_{\Gamma}$$
 (gauge *invariant*) (1.45b)

$$\mathcal{F}'_{lm} = \mathcal{F}_{lm}$$
 (gauge *invariant*) (1.45c)

11 | This motivates the following definition:

***** Definition: Berry phase

For n = 1, the exponent of the Berry holonomy is called ** *Berry phase*:

$$\gamma(\Gamma) = -\oint_{\Gamma} \mathcal{A} d\Gamma = i \oint_{\Gamma} \langle v(\Gamma) | \partial_{\Gamma_l} | v(\Gamma) \rangle d\Gamma_l \quad \in \mathbb{R}$$
(1.46)

The nomenclature is sometimes a bit vague: $\gamma(\Gamma)$ and $e^{i\gamma(\Gamma)}$ are both called "Berry phase."

- The Berry phase is a * geometric phase as compared to the usual \checkmark dynamical phases accumulated by wave functions in quantum mechanics. Remember that an eigenstate with energy E collects the phase $e^{-\frac{i}{\hbar}E\Delta t}$ in the time interval Δt due to the unitary evolution governed by the Schrödinger equation. Such phases are called dynamical phases. By contrast, the Berry phase is *not* a consequence of the energy of the system (recall that we set the ground state energy to zero for all parameters!); it is rather a geometric property of the parametric path Γ over the \uparrow vector bundle \mathcal{V} of ground state spaces.
- The Berry phase was first discussed by MICHAEL BERRY in 1984 [69].
- The Berry phase follows from the Berry connection. But where does the Berry connection "come from"? It seems that it is somehow hidden in the Hamiltonian family H(Γ), but this can only be partially true as the latter only defines a projector onto its ground state manifold. This provides us with the Hilbert sub-bundle V(Γ) on which the Berry connection is defined. But a projection does not magically produce a connection. Actually, we start from the full Hilbert bundle (its fibers are the Hilbert spaces on which the Hamiltonians act) und (silently) assume that it is trivialized M × H₀ with some reference Hilbert space H₀. A trivialized bundle has a natural connection, namely the trivial (or constant) connection. Starting from this connection, the ground state projection provided by a Hamiltonian then induces a connection on the sub-bundle V(Γ) and this is the Berry connection. If there is no canonical (or physically motivated) trivialization of the full Hilbert bundle, the choice of the connection on this bundle leads to potentially distinct Berry connections and thereby distinct Berry phases; for details on this subtlety see Ref. [66].
- **12** | Examples of systems with non-trivial Berry phase:
 - Spin-¹/₂ in a variable magnetic field (⇒ Problemset 2 and ↑ Ref. [69])
 - Aharonov-Bohm effect (1 [69])
 - Focault pendulum (^ [70,71])

The concept of parallel transport with non-trivial holonomies is not restricted to quantum mechanical systems!



13 $| \triangleleft$ Effect of gauge transformations on the Berry phase:

$$\gamma'(\Gamma) = -\oint_{\Gamma} \mathcal{A}' d\Gamma = -\oint_{\Gamma} (\mathcal{A} + \nabla_{\Gamma} \xi) d\Gamma = \gamma(\Gamma) - [\xi(\Gamma(T)) - \xi(\Gamma(0))] \quad (1.47)$$

Note that here $\xi(\Gamma(T))$ should be read as $\lim_{\varepsilon \to 0} \xi(\Gamma(T - \varepsilon))$ and $\xi(\Gamma(0))$ is shorthand for $\lim_{\varepsilon \to 0} \xi(\Gamma(0 + \varepsilon))$, which explains why Eq. (1.48) below makes sense even though $\Gamma(T) = \Gamma(0)$.

Continuity of the gauge transformation: $\Omega(\Gamma(0)) = \Omega(\Gamma(T)) \rightarrow$

Recall that Γ is a closed path: $\Gamma(T) = \Gamma(0)$. Note that continuity of the gauge transformation $e^{i\xi(\Gamma(0))} = \Omega(\Gamma(0)) = \Omega(\Gamma(T)) = e^{i\xi(\Gamma(T))}$ does not imply continuity of $\xi(\Gamma)$!

Eq. (1.45b)
$$\Rightarrow \xi(\Gamma(T)) - \xi(\Gamma(0)) = 2\pi m \text{ for } m \in \mathbb{Z}$$
 (1.48)

- $\rightarrow \gamma(\Gamma)$ is gauge invariant up multiples of 2π
- \rightarrow For $\gamma(\Gamma) \notin 2\pi\mathbb{Z}$, the Berry phase *cannot* be gauged away and can have physical consequences!

14 |
$$\triangleleft$$
 Special case k=2: $\Gamma = (\Gamma_1, \Gamma_2)$

This is the most important case for us because the parameter space we are interested in will be the 2D + Brillouin zone (which is a torus).

 \rightarrow Computation of the Berry phase for k = 2 on a compact manifold \mathcal{M} (sphere, torus):

i $| \triangleleft \text{Closed path } \Gamma \text{ on sphere } \mathcal{M} = S^2$ $\triangleleft \text{Submanifolds with } \Sigma \cup \overline{\Sigma} = \mathcal{M} \text{ and } \partial \Sigma = \Gamma = \partial \overline{\Sigma}$:



i! Important

In general it is *not* possible to choose a gauge that is continuous (= non-singular) everywhere on \mathcal{M} !

Hence we must be careful when integrating the Berry connection \mathcal{A} along paths on \mathcal{M} ! In the following, we assume that we *can* find continuous gauges for every simply connected, open submanifold of \mathcal{M} though:

ii | \triangleleft Continuous gauge $\mathcal{A}_1 \ \underline{\text{on } \Sigma} \rightarrow \text{Stokes' theorem valid on } \Sigma \rightarrow$

$$\oint_{\Gamma} \mathcal{A}_1 d\Gamma \stackrel{\text{Stokes}}{=} \int_{\Sigma} \mathcal{F}_{lm} d\sigma^{lm}$$
(1.49)

 σ^{lm} is the differential area element (a 2-form that is antisymmetric in l and m, just as \mathcal{F}_{lm}). For a reformulation in terms of differential forms see the comments \rightarrow *below*.



iii | \triangleleft Continuous gauge $A_2 \text{ on } \overline{\Sigma} \rightarrow$ Stokes' theorem valid on $\overline{\Sigma} \rightarrow$

$$\oint_{\Gamma} \mathcal{A}_2 \mathrm{d}\Gamma \stackrel{\mathrm{Stokes}}{=} -\int_{\bar{\Sigma}} \mathcal{F}_{lm} \mathrm{d}\sigma^{lm}$$
(1.50)

The sign is due to the opposite orientation of the boundary for $\overline{\Sigma}$.

iv | Using Eq. (1.48) \wedge Eq. (1.49) \wedge Eq. (1.50) \rightarrow

$$\int_{\mathcal{M}} \mathcal{F}_{lm} \mathrm{d}\sigma^{lm} = \underbrace{\oint_{\Gamma}}_{\gamma(\Gamma)+2\pi m_1} - \underbrace{\oint_{\Gamma}}_{\gamma(\Gamma)+2\pi m_2} \mathcal{A}_2 \mathrm{d}\Gamma = 2\pi m \quad \text{with} \quad m \in \mathbb{Z}$$
(1.51)

Here we used that the closed loop integrals of the Berry connection are unique up to integer multiples of 2π .

15 | This motivates the following definition:

***** Definition: Chern number

For a compact, closed two-dimensional parameter space \mathcal{M} with Berry curvature \mathcal{F} , the $\stackrel{*}{\ast}$ (*first*) Chern number is an integer and defined as

$$C := \frac{1}{2\pi} \int_{\mathcal{M}} \mathcal{F}_{lm} \mathrm{d}\sigma^{lm} \quad \in \mathbb{Z}$$
(1.52)

This is our first example of a *topological invariant*.

- We will meet the Chern number again in Section 1.4 where we compute the Hall conductivity.
- i! Following the argument above, it is clear that whenever there exists a gauge that is non-singular on the *complete* parameter space, the Chern number is necessarily zero. [Because you can then choose A₁ = A₂ such that the difference in Eq. (1.51) vanishes.] Conversely, whenever the Chern number does *not* vanish, there must be singularities in all gauges! You will encounter an example of this in S Problemset 2.

16 | ‡ Comments:

• Differential forms:

The proper way to formulate the application of Stokes' theorem is in terms of *differential forms*. In this framework

$$\mathcal{A} := \sum_{l=1}^{k} \mathcal{A}_l \mathrm{d}\Gamma_l \tag{1.53}$$

is a *1-form* that can be integrated along paths:

$$\gamma(\Gamma) = -\oint_{\Gamma} \mathcal{A} \,. \tag{1.54}$$

The Berry curvature is then the *2-form* given by the *exterior derivative* of A (this is only true for n = 1, i.e., abelian gauge fields):

$$\mathcal{F} := \mathrm{d}\mathcal{A} = \sum_{1 \le l, m \le k} \underbrace{(\partial_m \mathcal{A}_l - \partial_l \mathcal{A}_m)}_{\mathcal{F}_{lm}} \underbrace{\frac{1}{2} \mathrm{d}\Gamma_m \wedge \mathrm{d}\Gamma_l}_{\mathrm{d}\sigma^{lm}} = \mathcal{F}_{lm} \mathrm{d}\sigma^{lm}$$
(1.55)



where the last expression is just a shorthand notation. (For *non-abelian* gauge fields it is $\mathcal{F} = d\mathcal{A} + \mathcal{A} \wedge \mathcal{A}$; note that \mathcal{A} is a 1-form with values in a non-abelian Lie algebra so that the wedge product does not vanish in general.)

Finally, Stoke's theorem for differential forms states that

$$\oint_{\Gamma=\partial\Sigma} \mathcal{A} = \int_{\Sigma} d\mathcal{A} = \int_{\Sigma} \mathcal{F} .$$
(1.56)

• Observation of the Berry phase:



→ Interference pattern: $I = |1 + e^{i\gamma(\Gamma)}|^2$ where $e^{i\gamma(\Gamma)} = e^{i\Omega/2}$ with solid angle $0 \le \Omega \le 4\pi$. You will calculate the dependency of the Berry phase on the solid angle traced out by the magnetic field in \bigcirc Problemset 2. This experiment was already proposed and studied by Berry in his original work [69].

To the best of my knowledge, there has been no experiment that implemented exactly Berry's proposal (due to experimental issues controlling additional dynamical phases). However, there have been multiple other experimental verifications of the Berry phase in quantum systems since its prediction in 1984 [72,73]. (Note that the historically first reporting [74] was later disputed [75] because it can be explained classically, without invoking quantum mechanics.)

• Geometric interpretation of the Berry curvature:

In general, the parameter space can be multi-dimensional. For obvious reasons we only draw two of them:



The Berry holonomy can be compared to the rotation of a vector when carried ("parallel transported") around a closed curve on a curved space (like the shown sphere). The analog to the \checkmark *Riemann curvature* is the Berry curvature, the role of the \checkmark *Levi-Civita connection* is played by the Berry connection. The Chern number equals the \uparrow *Euler characteristic* of a compact 2D manifold, and the relation that gives the Chern number in terms of the



Berry curvature is then known as \uparrow *Gauss-Bonnet theorem* (more precisely: \uparrow *Chern-Gauss-Bonnet theorem*, a generalization of the classic Gauss-Bonnet theorem to even-dimensional Riemannian manifolds). This "real space analog" may be known from your lectures on \downarrow general relativity. Note that in general relativity one is interested in the \uparrow *tangent bundle* where a tangential space is attached to every point of the (spacetime) manifold. Here we are *not* interested in the tangent bundle of the parameter manifold but more general \uparrow *fiber bundles* where the local fibers are given by ground state spaces $\mathcal{V}(\Gamma)$ or Lie groups U(n) that act on them.

1.4. Quantization of the Hall conductivity

With these new mathematical insights, we now return to the integer quantum Hall effect and its Hall plateaus. Our goal is to find a relation between the Hall conductivity and the Chern number. This remarkable relation between a *physical quantity* and a *topological invariant* is one of the most important insights in contemporary condensed matter physics and explains the quantization of the Hall conductivity.

The following discussion is based on David Tong's lecture notes on the quantum Hall effect [64]. For a more detailed (and much more technical) discussion, see Chapter 3 of Bernevig's textbook [1]; another account can be found in Chapter 12 of Fradkin's textbook [63]. You might also want to have a look at the original manuscript by Thouless *et al.* [17] and the follow-up [76].

1.4.1. The Kubo formula

As a preparation, we compute the linear response of a quantum mechanical system at T = 0 for a time-dependent, external perturbation. Here we focus on the special case where the perturbation is a time-dependent electric field and the response is a current of charged particles. The approach is generic and valid for general (in particular: interacting) Hamiltonians. The resulting \rightarrow *Kubo formula* has many applications beyond computing the quantized Hall conductivity.

- 1 \triangleleft Unperturbed Hamiltonian H_0 with Eigenstates $|m\rangle$ and Eigenenergies E_m
 - \triangleleft Time-dependent perturbation $\Delta H(t)$
 - $\rightarrow H(t) = H_0 + \Delta H(t)$ (Schrödinger picture!)
- 2 | It is convenient to absorb the unperturbed time evolution into operators:
 - $\rightarrow \downarrow$ Interaction picture:

$$\Delta H_I(t) := U_0^{\dagger}(t) \Delta H(t) U_0(t) \quad \text{and} \quad |\Psi(t)\rangle_I := U(t, t_0) |\Psi(t_0)\rangle_I \tag{1.57}$$

with unperturbed time evolution operator $U_0(t) := e^{-\frac{t}{\hbar}H_0t}$ and

$$U(t,t_0) := \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_{t_0}^t \Delta H_I(t') dt'\right]$$
(1.58)

Here \mathcal{T} denotes the time-ordered exponential. It is easy to check that the states $|\Psi(t)\rangle_I$ satisfy the Schrödinger equation in the interaction picture:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle_I = \Delta H_I(t)|\Psi(t)\rangle_I.$$
 (1.59)

To show the unitary equivalence between the interaction picture and the conventional Schrödinger picture, you must show that $U(t, t_0) \stackrel{\circ}{=} U_0^{\dagger}(t - t_0)U_S(t, t_0)$ with the full Schrödinger evolution

$$U_S(t,t_0) := \mathcal{T} \exp\left[-\frac{i}{\hbar} \int_{t_0}^t H(t') dt'\right].$$
(1.60)

- **3** Prepare system for $t_0 \rightarrow -\infty$ in ground state $|0\rangle$ of H_0 (or some other eigenstate)
- **4** | \triangleleft Expectation value of arbitrary (interaction picture) operator $\mathcal{O}_I(t) = U_0^{\dagger} \mathcal{O} U_0$:

$$\langle \mathcal{O}(t) \rangle = \underbrace{\langle 0 | U_{S}^{\dagger}(t, -\infty) \mathcal{O} U_{S}(t, -\infty) | 0 \rangle}_{\text{Schrödinger picture}}$$
(1.61a)

$$=\underbrace{\langle 0|U^{\dagger}(t,-\infty)\mathcal{O}_{I}(t)U(t,-\infty)|0\rangle}_{\text{Interaction picture}}$$
(1.61b)

$$\stackrel{1.58}{\approx} \langle 0| \left\{ \mathcal{O}_{I}(t) + \frac{i}{\hbar} \int_{-\infty}^{t} \left[\Delta H_{I}(t'), \mathcal{O}_{I}(t) \right] \mathrm{d}t' \right\} | 0 \rangle$$
(1.61c)

This linearization is the core of *linear response* theory.

Note that time ordering is not important in linear order (only one time integral!).

 \rightarrow

** Kubo formula:

$$\delta\langle\mathcal{O}(t)\rangle \equiv \langle\mathcal{O}(t)\rangle - \langle\mathcal{O}\rangle = \frac{i}{\hbar} \int_{-\infty}^{t} \langle 0| \left[\Delta H_{I}(t'), \mathcal{O}_{I}(t)\right] |0\rangle dt' \qquad (1.62)$$

- This is the linear response of the system to the perturbation ΔH(t). Note that ⟨Ø⟩ = ⟨0|Ø|0⟩ = ⟨0|Ø_I(t)|0⟩ is not a dynamic response but the static expectation value of Ø in the initial state (remember that |0⟩ is a eigenstate of H₀). In the following, we will set it to zero.
- The Kubo formula was first presented by RYOGO KUBO in 1957 [77].