Topological Insulators

— Basics of Topological Insulators —

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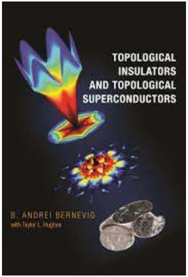
Outline

References

1. B. Andrei Bernevig, “Topological Insulators and Topological Superconductors” (Princeton, 2013)

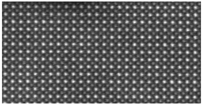
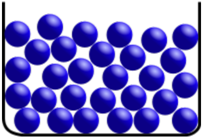
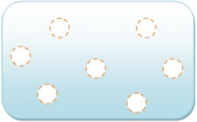
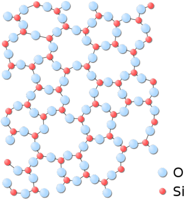


2. Shun-Qing Shen, “Topological Insulators: Dirac Equation in Condensed Matter” (Springer, 2012)
3. M. Z. Hasan and C. L. Kane, “Colloquium: Topological Insulators,” Review of Modern Physics **82**, 3045 (2010).
4. Xiao-Liang Qi and Shou-Cheng Zhang, “Topological insulators and superconductors,” Review of Modern Physics **83**, 1057 (2011).

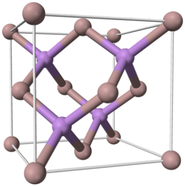
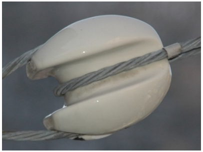
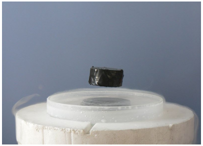
Outline

Phases

- solid, liquid, gas, glass

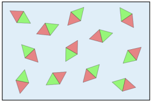
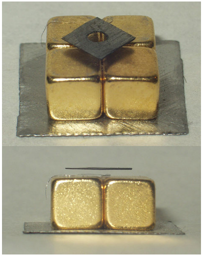





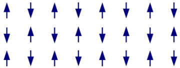
- conductor, semiconductor, insulator, superconductor

Phases (cont.)

- paramagnetism, diamagnetism, ferromagnetism, antiferromagnetism



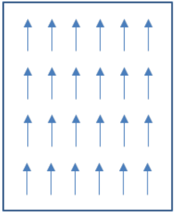
- charge-density wave, Bose-Einstein condensates

Phases (cont.)

- underlying principle for characterizing the state:

symmetry breaking and order parameter

- example: ferromagnetism



Ferromagnetic ordering

$$m = \frac{1}{N} \sum_{i=1}^{N} \langle S_z \rangle$$

breaking of the rotational symmetry of spins $\rightarrow$ finite magnetization $m \neq 0$

Phases (cont.)

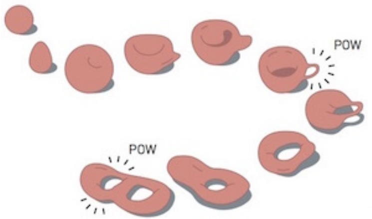
- Landau-Ginzburg theory ($\rightarrow$ phenomenological explanation of the phase transition): expansion of the free energy with respect to the order parameter

$$f(m) = \sum_{n=0}^{\infty} f_n m^n$$

  $\leftarrow$ order parameter can be very small near the phase transition
  - high-temperature symmetric phase
    $\Rightarrow$ low-temperature, less-symmetric, symmetry-broken state
  - first/second/$\cdots$-order transitions: depending on the vanishing of the second, third, $\cdots$ coefficient of the expansion of the free energy.
- major limitation of Landau-Ginzburg theory $\Leftarrow$ local order parameter

Topological States

- topology



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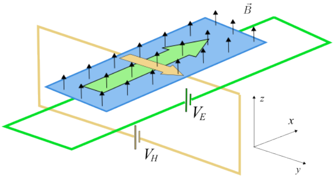
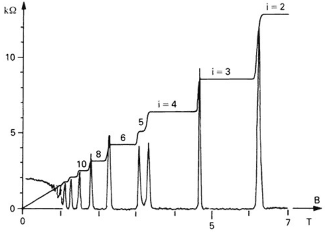
Topological States (cont.)

- phases of matter with topological order which cannot be described by a local order parameter
  - highly nonlocal order parameter
  - no Landau-like theory can be established
- example: quantum Hall states, quantum spin Hall states





$$\sigma_H = n\frac{e^2}{h}$$

Here n is the number of “holes” or magnetic monopoles of the fictitious magnetic field, so called the Berry field.

- topological phase = a phase of matter whose low-energy field theory is a topological field theory, or the states with nonlocal order parameter

Practical Application of Topological Phase

- topological quantum computer: example of Majorana fermion
  - » quantum qubits, $|0\rangle$ and $|1\rangle = c^\dagger |0\rangle$ defined by a single fermion
  - » single fermion operator (c) $\leftrightarrow$ two Majorana fermion operators (γ_1, γ_2)

$$\begin{aligned} \gamma_1 &= c^\dagger + c \\ \gamma_2 &= i(c^\dagger - c) \end{aligned} \quad \leftrightarrow \quad \begin{aligned} c &= \frac{\gamma_1 + i\gamma_2}{2} \\ c^\dagger &= \frac{\gamma_1 - i\gamma_2}{2} \end{aligned}$$

  - » how can the fermion c be nontrivial?

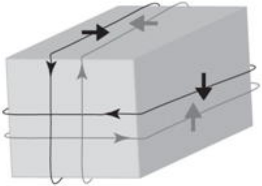
    1. γ_1 and γ_2 localize arbitrarily far apart from each other
       $\rightarrow$ c becomes a highly non-local operator
       $\rightarrow$ the occupation of c operator cannot be measured locally

$$c^\dagger c = \frac{1 + i\gamma_1\gamma_2}{2}$$

       $\rightarrow$ the fermionic state ($|0\rangle$ or $|1\rangle$) cannot be disturbed by a local perturbation
       $\rightarrow$ less susceptible to local decoherence processes
    2. one can empty or fill the non-local state with no energy cost, resulting in a ground-state degeneracy $\rightarrow$ non-Abelian statistics or braiding

Topological Band Theory

- Mostly, non-interacting fermionic systems
- existence of bulk invariant (usually an integer or a rational number or set of numbers) that differentiates between phases of matter having the same symmetry
- usually, but not always, topological states are associated with the existence of gapless edge modes

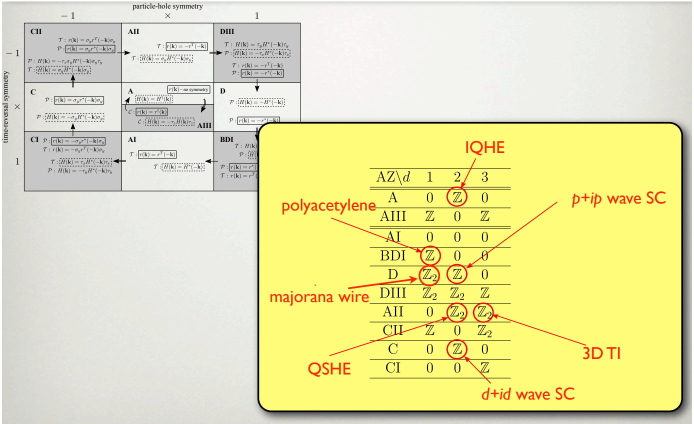


note that topological phases can exist without the presence of gapless edge modes.

- topological band theory takes into account concepts such as Chern numbers and Berry phases.
- in topological band theory, an important consideration is not only which symmetries the states breaks, but which symmetries must be preserved to ensure the stability of the topological state: symmetry-protected topological state

Topological Band Theory (cont.)

- periodic table classifying the (non-interacting) topological insulators/superconductors



considered symmetries: (1) time-reversal symmetry, (2) particle-hole symmetry (charge conjugation), and (3) chiral symmetry

- for every discrete symmetry, there must exist topological insulating phases with distinct physical properties and a topological number.

Topological Band Theory (cont.)

- identification of topological phase
  - trivial insulator = insulator that, upon slowly turning off the hopping elements between orbitals on different sites, flows adiabatically into the atomic limit
  - in many cases, the nontrivial topology $\rightarrow$ presence of gapless edge states in the energy spectrum of a system with boundaries
  - topological phase can theoretically exist without exhibiting gapless edge modes $\rightarrow$ the energy spectrum alone (with or without boundaries) is insufficient to determine the full topological character
    $\rightarrow$ topological structure is encoded in the eigenstates
  - "entanglement" (depends only on the eigenstates) $\rightarrow$ topological nature
    for example, topological entanglement entropy

Outline

Berry Phase

- quantum adiabatic transport in slowly varying (electric, magnetic, strain) fields
  $\rightarrow$ modification of the wave function by terms other than just the dynamical phase
  $\Rightarrow$ Berry phase
- adiabatic transport in Bloch-periodic systems — parameters (Bloch momenta $\mathbf{k}$) are varied in closed loops (bands or Fermi surfaces) by applying the electric field
- Here we derive the Berry phase for a particle obeying Hamiltonian evolution under a set of slowly varying parameters
  $\rightarrow$ the basis for defining a series of topological invariants (Chern numbers, Z_2 invariants, etc)

Outline

Berry Phase, Berry Vector Potential

- general Hamiltonian $\mathcal{H}(\mathbf{R}) = \mathcal{H}(\mathbf{R}(t))$ for time-varying parameters $\mathbf{R} = (R_1, R_2, R_3, \cdots)$ where $R_i = R_i(t)$
- adiabatic evolution — $\mathbf{R}(t)$ are varied very slowly (compared to other energy scales, for example, gaps) along a (open or closed) path $\mathcal{C}$ in the parameter space
- instantaneous orthonormal basis, $|n(\mathbf{R})\rangle$ at each $\mathbf{R}$

$$\mathcal{H}(\mathbf{R})\,|n(\mathbf{R})\rangle = E_n(\mathbf{R})\,|n(\mathbf{R})\rangle\,, \qquad \langle n(\mathbf{R})|m(\mathbf{R})\rangle = \delta_{nm} \tag{1}$$

- gauge in $|n(\mathbf{R})\rangle$
  - » $|n(\mathbf{R})\rangle$ is defined up to a phase (in the case of degenerate states, a matrix) $\rightarrow$ gauge freedom
  - » choice of a gauge $\rightarrow$ the phase of each basis function $|n(\mathbf{R})\rangle$ varies smoothly and is single-valued along the path $\mathcal{C}$
  - » in some cases, a smooth and single-valued choice is not possible along a closed path $\mathcal{C}$
  - » at least, smooth and single-valued gauges can be found piecewise in finite neighborhoods of the parameter space.

Berry Phase, Berry Vector Potential (cont.)

- adiabatic theorem $\rightarrow$ a system starting in an eigenstate $|n(\mathbf{R}(0))\rangle$ stays as an instantaneous eigenstate of the Hamiltonian $|n(\mathbf{R}(t))\rangle$ throughout the process. BUT what is the phase?
- Berry phase: time evolution of a wavefunction $|\psi(t)\rangle$ of a system prepared in an initial pure eigenstate $|n(\mathbf{R}(0))\rangle$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t E_n(\mathbf{R}(t'))dt'} e^{i\gamma_n} |n(\mathbf{R}(t))\rangle \tag{2}$$

1. conventional dynamical phase: $\frac{1}{\hbar}\int_0^t E_n(\mathbf{R}(t'))dt'$
2. Berry phase γ_n for the state n

$$\gamma_n = i\int_0^t \langle n(\mathbf{R}(t'))|\frac{d}{dt'}|n(\mathbf{R}(t'))\rangle\, dt' \tag{3}$$

Note that the Berry phase comes from the fact that $|n(\mathbf{R}(t))\rangle$ and $|n(\mathbf{R}(t+dt))\rangle$ are not identical

TI-1: proof of Eq. (2)

Berry Phase, Berry Vector Potential (cont.)

TI-1: proof of Eq. (2)

Let $\theta(t)$ be the phase of the state $|\psi(t)\rangle$ during the adiabatic evolution of the system so that

$$|\psi(t)\rangle = e^{-i\theta(t)} |n(\mathbf{R}(t))\rangle \qquad \text{(a)}$$

Note that $\theta(t)$ cannot be zero because it must at least contain the dynamical factor related to the energy of the eigenstate. By inserting Eq. (a) into the Schrödinger equation,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \mathcal{H}(\mathbf{R}(t)) |\psi(t)\rangle$$

one obtains the differential equation

$$\hbar \frac{d\theta(t)}{dt} e^{-i\theta(t)} |n(\mathbf{R}(t))\rangle + i\hbar e^{-i\theta(t)} \frac{d}{dt} |n(\mathbf{R}(t))\rangle = e^{-i\theta(t)} \mathcal{H}(\mathbf{R}(t)) |n(\mathbf{R}(t))\rangle$$

$$\hbar \frac{d\theta(t)}{dt} |n(\mathbf{R}(t))\rangle + i\hbar \frac{d}{dt} |n(\mathbf{R}(t))\rangle = E_n(\mathbf{R}(t)) |n(\mathbf{R}(t))\rangle$$

By taking the scalar product with $\langle n(\mathbf{R}(t))|$,

$$\hbar \frac{d\theta(t)}{dt} + i\hbar \langle n(\mathbf{R}(t))| \frac{d}{dt} |n(\mathbf{R}(t))\rangle = E_n(\mathbf{R}(t))$$

By integrating over time t, the solution for $\theta(t)$ is

$$\theta(t) = \underbrace{\frac{1}{\hbar} \int_0^t E_n(\mathbf{R}(t'))dt'}_{=\text{ dynamical phase}} - \underbrace{i \int_0^t \langle n(\mathbf{R}(t'))| \frac{d}{dt'} |n(\mathbf{R}(t'))\rangle}_{=\gamma_n}$$

Berry Phase, Berry Vector Potential (cont.)

- Berry connection or Berry vector potential $\mathbf{A}_n(\mathbf{R})$

$$\gamma_n = \int_{\mathcal{C}} d\mathbf{R} \cdot \mathbf{A}_n(\mathbf{R}) \quad \text{with} \quad \mathbf{A}_n(\mathbf{R}) \equiv i \langle n(\mathbf{R}) | \boldsymbol{\nabla}_{\mathbf{R}} | n(\mathbf{R}) \rangle \tag{4}$$

TI-2: proof of Eq. (4)

- Berry phase γ_n is real

$$\gamma_n = -\operatorname{Im} \int_{\mathcal{C}} d\mathbf{R} \cdot \langle n(\mathbf{R}) | \boldsymbol{\nabla}_{\mathbf{R}} | n(\mathbf{R}) \rangle \tag{5}$$

TI-3: proof of Eq. (5)

Berry Phase, Berry Vector Potential (cont.)

TI-2: proof of Eq. (4)

Since

$$\frac{d}{dt'}\left|n(\mathbf{R}(t'))\right\rangle = \frac{d}{dt'}\left|n(R_1(t'), R_2(t'), \cdots)\right\rangle = \sum_i \frac{\partial}{\partial R_i}\left|n(\mathbf{R})\right\rangle \frac{dR_i}{dt'} = \boldsymbol{\nabla}\left|n(\mathbf{R})\right\rangle \cdot \frac{d\mathbf{R}}{dt'}$$

the time can be removed explicitly from the equation

$$\begin{aligned}\gamma_n &= i\int_0^t \langle n(\mathbf{R}(t'))|\frac{d}{dt'}|n(\mathbf{R}(t'))\rangle\, dt' = i\int_0^t \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot \frac{d\mathbf{R}}{dt'}dt' \\ &= i\int_{\mathcal{C}} \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot d\mathbf{R}\end{aligned}$$

Berry Phase, Berry Vector Potential (cont.)

TI-3: proof of Eq. (5)

Since $\langle n(\mathbf{R})|n(\mathbf{R})\rangle = 1$, by differentiating with respect to $\mathbf{R}$,

$$0 = \langle \boldsymbol{\nabla}_{\mathbf{R}} n(\mathbf{R})|n(\mathbf{R})\rangle + \langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle$$
$$\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle = -\langle \boldsymbol{\nabla}_{\mathbf{R}} n(\mathbf{R})|n(\mathbf{R})\rangle = -\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle^*$$

Therefore, $\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle$ is purely imaginary, or $\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle = i\,\mathrm{Im}\,\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle$. So,

$$\gamma_n = i\int_{\mathcal{C}} d\mathbf{R}\cdot\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle = -\,\mathrm{Im}\int_{\mathcal{C}} d\mathbf{R}\cdot\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle$$

Berry Phase, Berry Vector Potential (cont.)

- γ_n and $\mathbf{A}_n(\mathbf{R})$ are gauge-dependent!

  Under gauge transformation, $|n(\mathbf{R})\rangle \to e^{i\zeta(\mathbf{R})}|n(\mathbf{R})\rangle$ with $\zeta(\mathbf{R})$ a smooth, single-valued function,

$$\begin{aligned} \mathbf{A}_n(\mathbf{R}) &\to \mathbf{A}_n(\mathbf{R}) - \nabla_{\mathbf{R}}\zeta(\mathbf{R}) \\ \gamma_n &\to \gamma_n + \zeta(\mathbf{R}(0)) - \zeta(\mathbf{R}(T)) \end{aligned} \tag{6}$$

  where T is the (long) time after which the path $\mathcal{C}$ has been completed.

TI-4: proof of Eq. (6)

  (note that the gauge dependence of $\mathbf{A}_n$ is similar to that of the vector potential of the "real" magnetic field)

- γ_n can be canceled by a smart choice of the gauge factor $\zeta(\mathbf{R})$? No!
- for closed path $\mathcal{C}$

$$\zeta(\mathbf{R}(0)) - \zeta(\mathbf{R}(T)) = 2\pi m \qquad \text{(for an integer } m\text{)} \tag{7}$$

  $\to$ the Berry phase cannot be canceled unless it is an integer itself.

TI-5: proof of Eq. (7)

For a closed path, the Berry phase is gauge-invariant quantity independent of the specific form of how $\mathbf{R}$ varies in time.

Berry Phase, Berry Vector Potential (cont.)

TI-4: proof of Eq. (6)

Under the gauge transformation,

$$\begin{aligned}\mathbf{A}_n &\to i\left(e^{-i\zeta(\mathbf{R})}\langle n(\mathbf{R})|\right)\boldsymbol{\nabla}_{\mathbf{R}}\left(e^{i\zeta(\mathbf{R})}|n(\mathbf{R})\rangle\right)\\ &= i\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle + i\langle n(\mathbf{R})|(i\boldsymbol{\nabla}_{\mathbf{R}}\zeta(\mathbf{R}))|n(\mathbf{R})\rangle\\ &= \mathbf{A}_n - \boldsymbol{\nabla}_{\mathbf{R}}\zeta(\mathbf{R})\end{aligned}$$

and

$$\begin{aligned}\gamma_n &\to \int_{\mathcal{C}} d\mathbf{R}\cdot(\mathbf{A}_n(\mathbf{R}) - \boldsymbol{\nabla}_{\mathbf{R}}\zeta(\mathbf{R}))\\ &= \gamma_n - \int_{\mathcal{C}} d\mathbf{R}\cdot\boldsymbol{\nabla}_{\mathbf{R}}\zeta(\mathbf{R})\\ &= \gamma_n - (\zeta(\mathbf{R}(T)) - \zeta(\mathbf{R}(0)))\end{aligned}$$

Berry Phase, Berry Vector Potential (cont.)

TI-5: proof of Eq. (7)

For closed path $\mathcal{C}$, after a long time T (period), we return to the original parameters:

$$\mathbf{R}(0) = \mathbf{R}(T)$$

(if R_i is angle variable, $R_i(0) = R_i(T)$ up to $2\pi m$ with an integer m). Since we have chosen our eigenstate basis to be single-valued,

$$|n(\mathbf{R}(0))\rangle = |n(\mathbf{R}(T))\rangle \tag{a}$$

Gauge transformation should maintain this property, so

$$e^{i\zeta(\mathbf{R}(0))}\,|n(\mathbf{R}(0))\rangle = e^{i\zeta(\mathbf{R}(T))}\,|n(\mathbf{R}(T))\rangle \tag{b}$$

From Eqs. (a) and (b), we have

$$e^{i\zeta(\mathbf{R}(0))} = e^{i\zeta(\mathbf{R}(T))}$$

or

$$\zeta(\mathbf{R}(0)) - \zeta(\mathbf{R}(T)) = 2\pi m$$

for integer m.

Berry Phase, Berry Vector Potential (cont.)

- for three-dimensional parameter space $\mathbf{R} = (R_1, R_2, R_3) = (R_x, R_y, R_z)$ and for a closed path $\mathcal{C}$

$$\gamma_n = -\operatorname{Im} \int_{\mathcal{S}} d\mathbf{S} \cdot \langle \boldsymbol{\nabla}_{\mathbf{R}} n(\mathbf{R})| \times |\boldsymbol{\nabla}_{\mathbf{R}} n(\mathbf{R})\rangle = \int_{\mathcal{S}} d\mathbf{S} \cdot \mathbf{F}_n(\mathbf{R}) \tag{8}$$

where $\mathcal{S}$ is an area enclosed by $\mathcal{C}$ and

$$F_{jk}(\mathbf{R}) \equiv i \left(\langle \nabla_j n(\mathbf{R}) | \nabla_k n(\mathbf{R}) \rangle - \langle \nabla_k n(\mathbf{R}) | \nabla_j n(\mathbf{R}) \rangle \right) \tag{9}$$

is defined to be Berry curvature which is the curl of the Berry vector potential, that is, a magnetic field in parameter space.

TI-6: proof of Eq. (8)

Note that the Berry curvature is gauge-independent:

$$\mathbf{F}_n(\mathbf{R}) \to \boldsymbol{\nabla}_{\mathbf{R}} \times (\mathbf{A}_n(\mathbf{R}) - \boldsymbol{\nabla}_{\mathbf{R}} \zeta(\mathbf{R})) = \boldsymbol{\nabla}_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R}) = \mathbf{F}_n(\mathbf{R})$$

- in this lecture, we consider only the case with closed path $\mathcal{C}$ and three-dimensional parameter space, $\dim(\mathbf{R}) = 3$.

Berry Phase, Berry Vector Potential (cont.)

TI-6: proof of Eq. (7)

Let $\mathcal{S}$ be the area enclosed by the closed path $\mathcal{C}$. Then, according to Stokes' theorem,

$$\begin{aligned}\gamma_n &= -\operatorname{Im}\int_{\mathcal{C}} d\mathbf{R}\cdot\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle = -\operatorname{Im}\int_{\mathcal{S}} d\mathbf{S}\cdot\boldsymbol{\nabla}\times\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}|n(\mathbf{R})\rangle \\ &= -\operatorname{Im}\int_{\mathcal{S}} dS_i\epsilon_{ijk}\nabla_j\langle n(\mathbf{R})|\nabla_k|n(\mathbf{R})\rangle \\ &= -\operatorname{Im}\int_{\mathcal{S}} dS_i\epsilon_{ijk}\left(\langle\nabla_j n(\mathbf{R})|\nabla_k|n(\mathbf{R})\rangle + \langle n(\mathbf{R})|\nabla_j\nabla_k|n(\mathbf{R})\rangle\right)\end{aligned}$$

Since $\epsilon_{ijk}\nabla_j\nabla_k = (\boldsymbol{\nabla}\times\boldsymbol{\nabla})_i = 0$, the second term vanishes. So,

$$\gamma_n = -\operatorname{Im}\int_{\mathcal{S}} dS_i\epsilon_{ijk}\langle\nabla_j n(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle = -\operatorname{Im}\int_{\mathcal{S}} d\mathbf{S}\cdot\langle\boldsymbol{\nabla}_{\mathbf{R}}n(\mathbf{R})|\times|\boldsymbol{\nabla}_{\mathbf{R}}n(\mathbf{R})\rangle$$

The curl of the Berry vector potential becomes

$$\begin{aligned}(\boldsymbol{\nabla}\times\mathbf{A}_n)_i = \epsilon_{ijk}\nabla_j A_{nk} = \epsilon_{ijk}\nabla_j i\langle n(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle &= \epsilon_{ijk} i\langle\nabla_j n(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle \\ &= \epsilon_{ijk} i\left(\langle\nabla_j n(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle - \langle\nabla_k n(\mathbf{R})|\nabla_j n(\mathbf{R})\rangle\right)\end{aligned}$$

where no summation over j and k in the last line

Outline

Another Formula for Berry Phase

- the derivative of the eigenstates, $\nabla_{\mathbf{R}} |n(\mathbf{R})\rangle$ in the expression of the Berry phase requires the gauge-smoothened eigenstates as functions of $\mathbf{R}$
- numerical diagonalization algorithm of $\mathcal{H}(\mathbf{R})$ usually outputs eigenstates with wildly (and randomly) different phase factors for different $\mathbf{R}$

→ a formula for the Berry phase that is gauge independent is demanded

- gauge-independent formula for the Berry phase

$$\gamma_n = -\int_{\mathcal{S}} d\mathbf{S} \cdot \mathbf{V}_n \tag{10}$$

with

$$\mathbf{V}_n \equiv \mathrm{Im} \sum_{m \neq n} \frac{\langle n(\mathbf{R})|\nabla_{\mathbf{R}}\mathcal{H}(\mathbf{R})|m(\mathbf{R})\rangle \times \langle m(\mathbf{R})|\nabla_{\mathbf{R}}\mathcal{H}(\mathbf{R})|n(\mathbf{R})\rangle}{[E_m(\mathbf{R}) - E_n(\mathbf{R})]^2} \tag{11}$$

Here $|n(\mathbf{R})\rangle$ is assumed to be nondegenerate.

TI-7: proof of Eq. (10)

Since the derivatives have been moved from the wavefunction to the Hamiltonian, the Berry curvature (or the Berry phase) can be evaluated under any gauge choice: it is no longer necessary to pick $|n(\mathbf{R})\rangle$ to be smooth and single-valued.

Another Formula for Berry Phase (cont.)

TI-7: proof of Eq. (10)

By introducing a complete set of eigenstates $\sum_m |m(\mathbf{R})\rangle\langle m(\mathbf{R})| = 1$ at each $\mathbf{R}$,

$$\begin{aligned}\epsilon_{ijk}\langle\nabla_j n(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle &= \epsilon_{ijk}\sum_m \langle\nabla_j n(\mathbf{R})|m(\mathbf{R})\rangle\langle m(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle \\ &= \epsilon_{ijk}\langle\nabla_j n(\mathbf{R})|n(\mathbf{R})\rangle\langle n(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle + \epsilon_{ijk}\sum_{m\neq n}\langle\nabla_j n(\mathbf{R})|m(\mathbf{R})\rangle\langle m(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle\end{aligned}$$

Note that $\langle\nabla_j n(\mathbf{R})|n(\mathbf{R})\rangle$ and $\langle n(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle$ are purely imaginary:

$$\begin{aligned}0 &= \nabla_j\langle n(\mathbf{R})|n(\mathbf{R})\rangle = \langle\nabla_j n(\mathbf{R})|n(\mathbf{R})\rangle + \langle n(\mathbf{R})|\nabla_j n(\mathbf{R})\rangle \\ \rightarrow \quad \langle\nabla_j n(\mathbf{R})|n(\mathbf{R})\rangle &= -\langle n(\mathbf{R})|\nabla_j n(\mathbf{R})\rangle = -\langle\nabla_j n(\mathbf{R})|n(\mathbf{R})\rangle^*\end{aligned}$$

Therefore, the first term is real and gives no contribution to the Berry phase (remember $\gamma_n = -\mathrm{Im}[\cdots]$). Hence,

$$\gamma_n = -\mathrm{Im}\int_{\mathcal{S}} dS_i \sum_{m\neq n}\epsilon_{ijk}\langle\nabla_j n(\mathbf{R})|m(\mathbf{R})\rangle\langle m(\mathbf{R})|\nabla_k n(\mathbf{R})\rangle \tag{a}$$

The derivative on the eigenstates can be removed in the following way:

$$E_n\langle m|\nabla n\rangle = \langle m|\nabla E_n|n\rangle = \langle m|\nabla|\mathcal{H}n\rangle = \langle m|(\nabla\mathcal{H})|n\rangle + \langle m|\mathcal{H}\nabla n\rangle = \langle m|(\nabla\mathcal{H})|n\rangle + E_m\langle m|\nabla n\rangle$$

Hence, since $E_n \neq E_m$ for $m \neq n$,

$$\langle m|\nabla n\rangle = \frac{\langle m|(\nabla\mathcal{H})|n\rangle}{E_n - E_m}$$

Another Formula for Berry Phase (cont.)

Similarly,

$$\langle \nabla n | m \rangle = \frac{\langle n | (\nabla \mathcal{H}) | m \rangle}{E_n - E_m}$$

By inserting the above two equations into Eq. (a),

$$\gamma_n = - \int_{\mathcal{S}} dS_i \, \mathrm{Im} \sum_{m \neq n} \epsilon_{ijk} \frac{\langle n(\mathbf{R}) | (\nabla_j \mathcal{H}) | m(\mathbf{R}) \rangle \langle m(\mathbf{R}) | (\nabla_k \mathcal{H}) | n(\mathbf{R}) \rangle}{[E_m(\mathbf{R}) - E_n(\mathbf{R})]^2} = - \int_{\mathcal{S}} dS_i V_{ni}$$

Another Formula for Berry Phase (cont.)

- two different equations for γ_n

$$\text{Eq. (8)} \rightarrow \quad \gamma_n = -\int_{\mathcal{S}} d\mathbf{S} \cdot \text{Im} \langle \nabla_{\mathbf{R}} n(\mathbf{R})| \times |\nabla_{\mathbf{R}} n(\mathbf{R})\rangle$$

$$\text{Eq. (10)} \rightarrow \quad \gamma_n = -\int_{\mathcal{S}} d\mathbf{S} \cdot \text{Im} \sum_{m \neq n} \frac{\langle n(\mathbf{R})|\nabla_{\mathbf{R}}\mathcal{H}(\mathbf{R})|m(\mathbf{R})\rangle \times \langle m(\mathbf{R})|\nabla_{\mathbf{R}}\mathcal{H}(\mathbf{R})|n(\mathbf{R})\rangle}{[E_m(\mathbf{R}) - E_n(\mathbf{R})]^2}$$

  » Eq. (8): involves only $|n(\mathbf{R})\rangle$ and its derivative
  » Eq. (10): involves the interaction between $|n(\mathbf{R})\rangle$ and $|m(\mathbf{R}) \neq n\rangle$ that have been projected out by the adiabatic interaction

- vanishing sum of the Berry phase

$$\sum_n \gamma_n = 0 \qquad (12)$$

TI-8: proof of Eq. (12)

- *d*-degenerate levels
  → the Berry vector potential becomes a matrix of dimension *d*
  → non-Abelian

Another Formula for Berry Phase (cont.)

TI-8: proof of Eq. (12)

Using Eq. (10)

$$\sum_n \gamma_n = -\int_{\mathcal{S}} d\mathbf{S} \cdot \sum_{n,m}^{n\neq m} \mathrm{Im}\, \frac{\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\mathcal{H}(\mathbf{R})|m(\mathbf{R})\rangle \times \langle m(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\mathcal{H}(\mathbf{R})|n(\mathbf{R})\rangle}{[E_m(\mathbf{R}) - E_n(\mathbf{R})]^2}$$

For any pair of (n, m),

$$\begin{aligned}
&\mathrm{Im}\, \frac{\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\mathcal{H}(\mathbf{R})|m(\mathbf{R})\rangle \times \langle m(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\mathcal{H}(\mathbf{R})|n(\mathbf{R})\rangle + (n \leftrightarrow m)}{[E_m(\mathbf{R}) - E_n(\mathbf{R})]^2} \\
&= \mathrm{Im}\, \frac{\langle n(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\mathcal{H}(\mathbf{R})|m(\mathbf{R})\rangle \times \langle m(\mathbf{R})|\boldsymbol{\nabla}_{\mathbf{R}}\mathcal{H}(\mathbf{R})|n(\mathbf{R})\rangle + (\text{complex conjugate})}{[E_m(\mathbf{R}) - E_n(\mathbf{R})]^2} \\
&= 0
\end{aligned}$$

Hence, $\sum_n \gamma_n = 0$.

Outline

Level Crossing

- Berry phase $\rightarrow$ classification of degeneracies
- at a degenerate point or level crossing ($E_n(\mathbf{R}) = E_m(\mathbf{R})$) at $\mathbf{R} = \mathbf{R}^*$, γ_n and γ_m diverge $\rightarrow$ $\mathbf{R}^* =$ a monopole in the parameter space
- here, the value of the Berry curvature at the degenerate point is not of our interest, but instead its global structure around the degenerate point is to be examined, which determines the Berry phase.
- generic degeneracy point at the intersection (at $\mathbf{R}^*$) of two levels as $\mathbf{R}$ is varies $\rightarrow$ two-level systems
  - two states $|\pm(\mathbf{R})\rangle$ with energy $E_\pm(\mathbf{R})$
  - $\mathbf{V}_+(\mathbf{R}) = -\mathbf{V}_-(\mathbf{R})$ and $\gamma_+ = -\gamma_-$
- generic form of two-level (or two-band) Hamiltonian

$$\mathcal{H} = \epsilon(\mathbf{R})\sigma_0 + \mathbf{d}(\mathbf{R}) \cdot \boldsymbol{\sigma} \tag{13}$$

  where σ_i are Pauli matrices ($i = 1, 2, 3$) and $\mathbf{d}(\mathbf{R})$ is a 3D vector depending on $\mathbf{R}$
  - $E_\pm = \epsilon(\mathbf{R}) \pm |\mathbf{d}(\mathbf{R})|$
  - $\epsilon(\mathbf{R})$ is just an additive term in energy and does not affect the eigenstates, being safely neglected.
  - examples: graphene, spin-orbit coupled systems, Bogoliubov quasiparticles, spin-$\frac{1}{2}$ electron in a magnetic field

Two-Level Systems Using the Berry Curvature

- parameterization by spherical coordinates

$$\mathbf{d}(\mathbf{R}) = \mathbf{d}(|d|, \theta, \phi) = |d|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{14}$$

- eigenvalues: $E_{\pm} = \pm|d|$
- eigenstates: at a choice of gauge (gauge 1)

$$|-(\mathbf{R})\rangle = \begin{bmatrix} e^{-i\phi}\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{bmatrix}, \quad |+(\mathbf{R})\rangle = \begin{bmatrix} e^{-i\phi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix} \tag{15}$$

or, at a different choice of gauge (gauge 2) (by $\times e^{+i\phi}$)

$$|-(\mathbf{R})\rangle = \begin{bmatrix} \sin\frac{\theta}{2} \\ -e^{+i\phi}\cos\frac{\theta}{2} \end{bmatrix}, \quad |+(\mathbf{R})\rangle = \begin{bmatrix} \cos\frac{\theta}{2} \\ e^{+i\phi}\sin\frac{\theta}{2} \end{bmatrix} \tag{16}$$

TI-9: proof of Eq. (15)

Two-Level Systems Using the Berry Curvature (cont.)

TI-9: proof of Eq. (15)

$$\mathcal{H}(\mathbf{R}) = |d| \begin{bmatrix} \cos\theta & \sin\theta\cos\phi - i\sin\theta\sin\phi \\ \sin\theta\cos\phi + i\sin\theta\sin\phi & -\cos\theta \end{bmatrix} = |d| \begin{bmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{+i\phi}\sin\theta & -\cos\theta \end{bmatrix}$$

The eigenvalues E are obtained from the secular equation

$$0 = (|d|\cos\theta - E)(-|d|\cos\theta - E) - |d|^2\sin^2\theta = E^2 - |d|^2 \quad \rightarrow \quad E = \pm|d|$$

For $E = +|d|$, the eigenstate satisfies

$$0 = (\mathcal{H} - |d|) \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = |d| \begin{bmatrix} \cos\theta - 1 & e^{-i\phi}\sin\theta \\ e^{+i\phi}\sin\theta & -\cos\theta - 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$= 2|d| \begin{bmatrix} -\sin^2\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ e^{+i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & -\cos^2\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \quad \rightarrow \quad \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} e^{-i\phi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix}$$

For $E = -|d|$, the eigenstate satisfies

$$0 = (\mathcal{H} + |d|) \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = |d| \begin{bmatrix} \cos\theta + 1 & e^{-i\phi}\sin\theta \\ e^{+i\phi}\sin\theta & -\cos\theta + 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$= 2|d| \begin{bmatrix} \cos^2\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ e^{+i\phi}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \quad \rightarrow \quad \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} e^{-i\phi}\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{bmatrix}$$

Two-Level Systems Using the Berry Curvature (cont.)

- Berry vector potentials A_θ and A_ϕ and Berry curvature $F_{\theta\phi}$ for level $|-(\mathbf{R})\rangle$
  1. gauge 1

$$A_\theta = 0, \quad A_\phi = +\sin^2\frac{\theta}{2}, \quad F_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = \frac{\sin\theta}{2} \tag{17}$$

  2. gauge 2

$$A_\theta = 0, \quad A_\phi = -\cos^2\frac{\theta}{2}, \quad F_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = \frac{\sin\theta}{2} \tag{18}$$

  Note that while the Berry vector potential is gauge-dependent, the Berry curvature is gauge-independent.

TI-10: proof of Eqs. (17) and (18)

Two-Level Systems Using the Berry Curvature (cont.)

TI-10: proof of Eqs. (17) and (18)

For gauge 1,

$$A_\theta = i\langle -(\mathbf{R})|\partial_\theta|-(\mathbf{R})\rangle = i\begin{bmatrix} e^{+i\phi}\sin\frac{\theta}{2} & -\cos\frac{\theta}{2}\end{bmatrix}\frac{1}{2}\begin{bmatrix} e^{-i\phi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}\end{bmatrix} = 0$$

$$A_\phi = i\langle -(\mathbf{R})|\partial_\phi|-(\mathbf{R})\rangle = i\begin{bmatrix} e^{+i\phi}\sin\frac{\theta}{2} & -\cos\frac{\theta}{2}\end{bmatrix}\begin{bmatrix} -ie^{-i\phi}\sin\frac{\theta}{2} \\ 0\end{bmatrix} = \sin^2\frac{\theta}{2}$$

$$F_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = \frac{1}{2}2\sin\frac{\theta}{2}\cos\frac{\theta}{2} = \frac{\sin\theta}{2}$$

For gauge 2,

$$A_\theta = i\langle -(\mathbf{R})|\partial_\theta|-(\mathbf{R})\rangle = i\begin{bmatrix} \sin\frac{\theta}{2} & -e^{-i\phi}\cos\frac{\theta}{2}\end{bmatrix}\frac{1}{2}\begin{bmatrix} \cos\frac{\theta}{2} \\ e^{+i\phi}\sin\frac{\theta}{2}\end{bmatrix} = 0$$

$$A_\phi = i\langle -(\mathbf{R})|\partial_\phi|-(\mathbf{R})\rangle = i\begin{bmatrix} \sin\frac{\theta}{2} & -e^{-i\phi}\cos\frac{\theta}{2}\end{bmatrix}\begin{bmatrix} 0 \\ -ie^{+i\phi}\cos\frac{\theta}{2}\end{bmatrix} = -\cos^2\frac{\theta}{2}$$

$$F_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = -\frac{1}{2}2\cos\frac{\theta}{2}\left(-\sin\frac{\theta}{2}\right) = \frac{\sin\theta}{2}$$

Two-Level Systems Using the Berry Curvature (cont.)

- the wavefunction $|-(\mathbf{R})\rangle$ is not well defined if the system reach, in its adiabatic evolution,

1. gauge 1: the south pole ($\theta = \pi$),

$$|-(\mathbf{R})\rangle = \begin{bmatrix} e^{-i\phi} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} \end{bmatrix} \rightarrow \begin{bmatrix} e^{-i\phi} \\ 0 \end{bmatrix}$$

2. gauge 2: the north pole ($\theta = 0$)

$$|-(\mathbf{R})\rangle = \begin{bmatrix} \sin \frac{\theta}{2} \\ -e^{+i\phi} \cos \frac{\theta}{2} \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ -e^{+i\phi} \end{bmatrix}$$

note that ϕ cannot be defined at $\theta = 0$ and π.

$\rightarrow$ In nontrivial cases, one cannot pick a gauge that is everywhere well defined. It is extremely important in the Chern insulator: if we are able to find a gauge in which all wavefunctions are well defined, then the system cannot have nonzero Hall conductance.

Two-Level Systems Using the Berry Curvature (cont.)

- For general $\mathbf{d}(\mathbf{R})$, (assuming $|d|$ is fixed)

$$F_{ij} = F_{\theta\phi}\frac{\partial(\theta,\phi)}{\partial(R_i,R_j)} = \frac{1}{2}\sin\theta\frac{\partial(\theta,\phi)}{\partial(R_i,R_j)} = -\frac{1}{2}\frac{\partial(\cos\theta,\phi)}{\partial(R_i,R_j)} = \frac{1}{2}\frac{\partial(\phi,\cos\theta)}{\partial(R_i,R_j)} \quad (19)$$

where the Jacobian is defined as $\dfrac{\partial(\theta,\phi)}{\partial(R_i,R_j)} \equiv \det\begin{bmatrix}\frac{\partial\theta}{\partial R_i} & \frac{\partial\theta}{\partial R_j} \\ \frac{\partial\phi}{\partial R_i} & \frac{\partial\phi}{\partial R_j}\end{bmatrix}$

- For $\mathbf{d}(\mathbf{R}) = \mathbf{R}$,

$$\mathbf{V}_- = -\frac{1}{2}\frac{\mathbf{R}}{R^3} = -\mathbf{V}_+ \quad (20)$$

TI-11: proof of Eq. (20)

  - degenerate point at $R = 0 \to$ field generated by a monopole (in $\mathbf{R}$ parameter space) of strength $\pm 1/2$ for band $|\pm(\mathbf{R})\rangle$
  - degenerate point = sources and drains of the Berry curvature

Two-Level Systems Using the Berry Curvature (cont.)

- example: integration of the Berry curvature over a sphere $\mathcal{S}$ containing the monopoles,

$$\gamma_n = -\int_{\mathcal{S}} d\mathbf{S} \cdot \mathbf{V}_- = \frac{1}{2} \times 4\pi n = 2\pi n \tag{21}$$

where n is the number of monopoles inside the surface $\mathcal{S}$ $\rightarrow$ Chern number.

Two-Level Systems Using the Berry Curvature (cont.)

TI-11: proof of Eq. (20)

For $\mathbf{d}(\mathbf{R}) = \mathbf{R}$,

$$|d|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) = (R_1, R_2, R_3)$$

so

$$\cos\theta = \frac{R_3}{R} = \frac{R_3}{\sqrt{R_1^2 + R_2^2 + R_3^2}} \quad \text{and} \quad \phi = \tan^{-1}\frac{R_2}{R_1}$$

Using

$$\frac{\partial\cos\theta}{\partial R_1} = -\frac{R_3 R_1}{R^3}, \quad \frac{\partial\cos\theta}{\partial R_2} = -\frac{R_3 R_2}{R^3}, \quad \frac{\partial\cos\theta}{\partial R_3} = \frac{1}{R} - \frac{R_3^2}{R^3} = \frac{R_1^2 + R_2^2}{R^3}$$

$$\frac{\partial\phi}{\partial R_1} = \frac{-R_2/R_1^2}{1 + (R_2/R_1)^2} = -\frac{R_2}{R_1^2 + R_2^2}, \quad \frac{\partial\phi}{\partial R_2} = \frac{1/R_1}{1 + (R_2/R_1)^2} = \frac{R_1}{R_1^2 + R_2^2}, \quad \frac{\partial\phi}{\partial R_3} = 0$$

one obtains

$$-V_{-1} = F_{23} = \frac{1}{2}\frac{\partial(\phi, \cos\theta)}{\partial(R_2, R_3)} = \frac{1}{2}\det\begin{bmatrix} \frac{R_1}{R_1^2+R_2^2} & 0 \\ -\frac{R_3 R_2}{R^3} & \frac{R_1^2+R_2^2}{R^3} \end{bmatrix} = \frac{1}{2}\frac{R_1}{R^3}$$

$$-V_{-2} = F_{31} = \frac{1}{2}\frac{\partial(\phi, \cos\theta)}{\partial(R_3, R_1)} = \frac{1}{2}\det\begin{bmatrix} 0 & -\frac{R_2}{R_1^2+R_2^2} \\ \frac{R_1^2+R_2^2}{R^3} & -\frac{R_3 R_1}{R^3} \end{bmatrix} = \frac{1}{2}\frac{R_2}{R^3}$$

$$-V_{-3} = F_{12} = \frac{1}{2}\frac{\partial(\phi, \cos\theta)}{\partial(R_1, R_2)} = \frac{1}{2}\det\begin{bmatrix} -\frac{R_2}{R_1^2+R_2^2} & \frac{R_1}{R_1^2+R_2^2} \\ -\frac{R_3 R_1}{R^3} & -\frac{R_3 R_2}{R^3} \end{bmatrix} = \frac{1}{2}\frac{R_2^2 R_3 + R_1^2 R_3}{R^3(R_1^2 + R_2^2)} = \frac{1}{2}\frac{R_3}{R^3}$$

Two-Level Systems Using the Hamiltonian Approach

- gauge-invariant approach, Eq. (10) $\rightarrow \nabla_{\mathbf{R}}\mathcal{H}$ is needed
- without loss of generality, by neglecting $\epsilon(\mathbf{R})$

$$\mathcal{H}(\mathbf{R}) = \mathbf{d}(\mathbf{R}) \cdot \boldsymbol{\sigma} \tag{22}$$

with the degeneracy point at $\mathbf{R}^* = 0$ (and $\mathbf{d}(\mathbf{R}^*) = 0$). Near the degenerate point, under an extra rotation, the Hamiltonian is linearized so that

$$\mathbf{d}(\mathbf{R}) = \mathbf{R} \qquad \text{near } \mathbf{R}^* \qquad \rightarrow \qquad \nabla_{\mathbf{R}}\mathcal{H} = \boldsymbol{\sigma} \tag{23}$$

and the eigenvalues are $E_\pm = \pm R$.

- Berry curvature for $|+(\mathbf{R})\rangle$

$$\mathbf{V}_+(\mathbf{R}) = \frac{1}{2}\frac{\mathbf{R}}{R^3} \tag{24}$$

TI-12: proof of Eq. (24)

- Berry phase

$$\gamma_\pm = -\int_{\mathcal{S}} d\mathbf{S} \cdot \mathbf{V}_\pm(\mathbf{R}) \quad \rightarrow \quad \exp[i\gamma_\pm(\mathcal{C})] = \exp\left[\mp\frac{1}{2}i\Omega(\mathcal{C})\right] \tag{25}$$

where $\Omega(\mathcal{C})$ is the solid angle that the surface $\mathcal{S}$ subtends at the degeneracy points.

Two-Level Systems Using the Hamiltonian Approach (cont.)

TI-12: proof of Eq. (24)

For easier calculation, we rotate the axes so that the z-axis points along $\mathbf{R}$. Then,

$$\mathcal{H}(\mathbf{R}) = R\sigma_z$$

so that the eigenstates are $|\pm\rangle$ which are the eigenstates of σ_z: $\sigma_z |\pm\rangle = \pm |\pm\rangle$. Note that $\sigma_x |\pm\rangle = |\mp\rangle$ and $\sigma_y |\pm\rangle = \pm i |\mp\rangle$. In this basis, from Eq. (10)

$$\mathbf{V}_n = \mathrm{Im} \sum_{m \neq n} \frac{\langle n(\mathbf{R})|\nabla_{\mathbf{R}}\mathcal{H}(\mathbf{R})|m(\mathbf{R})\rangle \times \langle m(\mathbf{R})|\nabla_{\mathbf{R}}\mathcal{H}(\mathbf{R})|n(\mathbf{R})\rangle}{[E_m(\mathbf{R}) - E_n(\mathbf{R})]^2}$$

one immediately knows that $V_{+x} = V_{+y} = 0$ because they involves the terms $\langle -|\sigma_z|+\rangle = 0$. The remaining term is then

$$V_{+z} = \mathrm{Im} \frac{\langle +|\sigma_x|-\rangle \langle -|\sigma_y|+\rangle - \langle +|\sigma_y|-\rangle \langle -|\sigma_x|+\rangle}{[E_-(\mathbf{R}) - E_+(\mathbf{R})]^2} = \mathrm{Im} \frac{i - (-i)}{4R^2} = \frac{R}{2R^3}$$

By rotating the system back in the original direction, the rotational invariance implies

$$\mathbf{V}_+(\mathbf{R}) = \frac{1}{2}\frac{\mathbf{R}}{R^3}$$

Two-Level Systems Using the Hamiltonian Approach (cont.)

- example: Dirac fermion (and Weyl fermion as well)
  - Hamiltonian

$$\mathcal{H} = \mathbf{k} \cdot \boldsymbol{\sigma} \tag{26}$$

    where **k** is the lattice momenta varying across the Brillouin zone.
  - what happens to the wavefunction of a Dirac fermion as it is transported around a path $\mathcal{C}$ in momentum space $\rightarrow$ acquire the Berry phase $\mp\frac{1}{2}\Omega(\mathcal{C})$.
  - 2D Dirac fermion $\rightarrow$ a closed path with $k_z = 0$

$$\Omega(\mathcal{C}) = \begin{cases} 2\pi, & \text{if the curve encircles the degeneracy} \\ 0, & \text{otherwise} \end{cases} \quad \rightarrow \quad e^{i\gamma_\pm(\mathcal{C})} = \begin{cases} -1 \\ +1 \end{cases} \tag{27}$$

    The Berry phase of the eigenstate of a gapless Dirac fermion in two dimensions have a Berry phase equal to π upon going around the Fermi surface.

Outline

Berry Phase

- Berry phase/curvature in solid-state physics $\leftarrow$ dimension, band structure
- Berry phase = integral of the Berry potential over a closed curve $\rightarrow$ 1D manifold
  1. filled bands (insulators) in 1D — $-\frac{\pi}{a} \leq k < \frac{\pi}{a} (= -\frac{\pi}{a})$ (a lattice spacing)
  2. Fermi surfaces of 2D metals
- Berry phase = surface integral of the Berry curvature (2-form) $\rightarrow$ 2D manifold
  1. filled bands (insulators) in 2D — full 2D Brillouin zone (BZ)
  2. Fermi surfaces of 3D metals $\rightarrow$ Chern number
- objective
  » Hall conductance of the 2D insulator
  $=$ the integral of the Berry curvature over the full BZ
  $=$ Chern number

$$\sigma_{xy} = \frac{e^2}{h} \frac{1}{2\pi} \int d\mathbf{k} \cdot \mathbf{F} \tag{28}$$

with

$$F_{xy}(\mathbf{k}) = \frac{\partial A_y(\mathbf{k})}{\partial k_x} - \frac{\partial A_x(\mathbf{k})}{\partial k_y} \quad \text{and} \quad \mathbf{A}(\mathbf{k}) = -i \sum_{\alpha \in \text{filled bands}} \langle \alpha \mathbf{k} | \boldsymbol{\nabla}_{\mathbf{k}} | \alpha \mathbf{k} \rangle \tag{29}$$

Outline

Current Operator in Continuum Model

- electrical current density in classical mechanics

$$\mathbf{J}_e(\mathbf{r}) = en(\mathbf{r})\mathbf{v}(\mathbf{r}) \tag{30}$$

  where $n(\mathbf{r})$ and $\mathbf{v}$ are number density and velocity of electrons.
- electrical current density operator in quantum mechanics

$$\mathbf{J}_e(\mathbf{r}) = \frac{e}{2}\sum_i [\mathbf{v}_i\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{v}_i] \equiv e\mathbf{J}(\mathbf{r}) \tag{31}$$

  - $\mathbf{r}_i$ and $\mathbf{v}_i = d\mathbf{r}_i/dt$ are position and velocity operators of particle i
  - in quantum mechanics, position and velocity operators do not commute $\rightarrow$ symmetrization

Current Operator in Continuum Model (cont.)

- current density operator in the presence of electromagnetic field

$$\begin{aligned}\mathbf{J}(\mathbf{r}) &= \frac{1}{2m}\sum_i \left[\left(\mathbf{p}_i - \frac{e}{c}\mathbf{A}(\mathbf{r}_i,t)\right)\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\left(\mathbf{p}_i - \frac{e}{c}\mathbf{A}(\mathbf{r}_i,t)\right)\right] \\ &= \mathbf{j}(\mathbf{r}) - \frac{e}{mc}\sum_i \mathbf{A}(\mathbf{r}_i,t)\delta(\mathbf{r}-\mathbf{r}_i)\end{aligned} \tag{32}$$

where $\mathbf{A}(\mathbf{r},t)$ is the vector potential.

» paramagnetic contribution (proportional to external field)

$$\mathbf{j}(\mathbf{r}) \equiv \frac{1}{2m}\sum_i [\mathbf{p}_i\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{p}_i] \tag{33}$$

» diamagnetic contribution (proportional to external field)

$$-\frac{e}{mc}n_0\mathbf{A}(\mathbf{r},t) \quad \rightarrow \quad \mathbf{J}_e(\mathbf{r},t) = \frac{in_0e^2}{m\omega}\mathbf{E}(\mathbf{r},t) \tag{34}$$

where n_0 is the uniform number density of charges.

TI-13: proof of Eq. (32)

Current Operator in Continuum Model (cont.)

TI-13: proof of Eq. (32)

In the presence of electromagnetic field, the Hamiltonian reads

$$\mathcal{H} = \sum_i \frac{1}{2m}\left(\mathbf{p}_i - \frac{e}{c}\mathbf{A}(\mathbf{r}_i, t)\right)^2 + \sum_i e\varphi(\mathbf{r}_i, t) + \sum_{i<j} V_{ij}(\mathbf{r}_i, \mathbf{r}_j)$$

where V_{ij} is electron-electron the interaction between particles. Then the velocity operator is given by (for $s = x, y, z$)

$$\begin{aligned} v_{is} = \frac{dr_{is}}{dt} &= \frac{i}{\hbar}[\mathcal{H}, r_{is}] = \frac{1}{2m}[\left(p_{is} - \frac{e}{c}A_s(\mathbf{r}_i, t)\right)^2, r_{is}] \\ &= \frac{i}{\hbar}\frac{1}{2m}\left[\left(p_{is} - \frac{e}{c}A_s(\mathbf{r}_i, t)\right)\underbrace{[p_{is}, r_{is}]}_{=-i\hbar} + \underbrace{[p_{is}, r_{is}]}_{=-i\hbar}\left(p_{is} - \frac{e}{c}A_s(\mathbf{r}_i, t)\right)\right] \\ &= \frac{1}{m}\left(p_{is} - \frac{e}{c}A_s(\mathbf{r}_i, t)\right) \end{aligned}$$

Current Operator in Continuum Model (cont.)

- external time-dependent external electric field

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)} \tag{35}$$

From

$$\mathbf{E} = -\boldsymbol{\nabla}\varphi - \frac{\partial \mathbf{A}}{\partial t} \quad \text{and} \quad \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} \tag{36}$$

and under the assumption that the electric field and vector potential are transverse,

$$\varphi(\mathbf{r}, t) = 0 \quad \text{and} \quad \mathbf{A}(\mathbf{r}, t) = \frac{\mathbf{E}(\mathbf{r}, t)}{i\omega} \tag{37}$$

- Hamiltonian in terms of current operator

$$\mathcal{H} = \mathcal{H}_0 - \frac{e}{c} \int d^3r \int \delta\mathbf{A}(\mathbf{r}, t) \cdot \mathbf{J}(\mathbf{r}) \tag{38}$$

where $\mathcal{H}_0$ is the Hamiltonian in the absence of electromagnetic field.

TI-14: proof of Eq. (38)

- weak electromagnetic field: up to the linear order in $\mathbf{A}(\mathbf{r}, t)$

$$\mathcal{H} = \mathcal{H}_0 - \frac{e}{c} \int d^3r \, \mathbf{A}(\mathbf{r}, t) \cdot \mathbf{j}(\mathbf{r}) \equiv \mathcal{H}_0 + \mathcal{H}_{\text{ext}} \tag{39}$$

Current Operator in Continuum Model (cont.)

TI-14: proof of Eq. (38)

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + \frac{1}{2m}\left[\mathbf{p}_i \cdot \left(-\frac{e}{c}\mathbf{A}(\mathbf{r}_i, t)\right) + \left(-\frac{e}{c}\mathbf{A}(\mathbf{r}_i, t)\right)\cdot \mathbf{p}_i + \frac{e^2}{c^2}A^2(\mathbf{r}_i, t)\right] \\
&= \mathcal{H}_0 - \frac{e}{c}\int d^3r \frac{1}{2m}\sum_i \left[\mathbf{p}_i \cdot \mathbf{A}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_i) + \mathbf{A}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_i)\cdot \mathbf{p}_i - \frac{e}{c}A^2(\mathbf{r}, t)\delta(\mathbf{r}-\mathbf{r}_i)\right] \\
&= \mathcal{H}_0 - \frac{e}{c}\int d^3r \int \delta\mathbf{A}(\mathbf{r}, t)\cdot \frac{1}{2m}\sum_i \left[\mathbf{p}_i\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{p}_i - 2\frac{e}{c}A(\mathbf{r}, t)\delta(\mathbf{r}-\mathbf{r}_i)\right] \\
&= \mathcal{H}_0 - \frac{e}{c}\int d^3r \int \delta\mathbf{A}(\mathbf{r}, t)\cdot \frac{1}{2m}\sum_i \left[\left(\mathbf{p}_i - \frac{e}{c}A(\mathbf{r}, t)\right)\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\left(\mathbf{p}_i - \frac{e}{c}A(\mathbf{r}, t)\right)\right] \\
&= \mathcal{H}_0 - \frac{e}{c}\int d^3r \int \delta\mathbf{A}(\mathbf{r}, t)\cdot \mathbf{J}(\mathbf{r})
\end{aligned}$$

Current Operator in Tight-Binding Model

- non-interacting tight-binding Hamiltonian

$$\mathcal{H} = \sum_{ij} \sum_{\alpha\beta} c_{i\alpha}^{\dagger} h_{ij}^{\alpha\beta} c_{j\beta} \tag{40}$$

  - i, j (or $\mathbf{r}_i$): lattice indices (sites) on arbitrary dimensional lattice — total N sites
  - α, β: orbital/spin indices — total M orbitals $\to$ M bands
  - $h_{ij}^{\alpha\beta} - \mu\delta_{ij}\delta_{\alpha\beta} \to h_{ij}^{\alpha\beta}$: zero chemical potential
  - translational symmetry

$$h_{ij}^{\alpha\beta} = h_{i-j}^{\alpha\beta} \tag{41}$$

- Fourier transform:

$$c_{\mathbf{k}\alpha} = \frac{1}{\sqrt{N}} \sum_{i} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{i\alpha} \quad \text{and} \quad c_{i\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\alpha} \tag{42}$$

$\to$

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{\alpha\beta} c_{\mathbf{k}\alpha}^{\dagger} h_{\mathbf{k}}^{\alpha\beta} c_{\mathbf{k}\beta} \tag{43}$$

TI-15: proof of Eq. (43)

Current Operator in Tight-Binding Model (cont.)

TI-15: proof of Eq. (43)

$$\mathcal{H} = \sum_{ij}\sum_{\alpha\beta} c^\dagger_{i\alpha} h^{\alpha\beta}_{ij} c_{j\beta} = \sum_{ij}\sum_{\alpha\beta} \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c^\dagger_{\mathbf{k}\alpha} h^{\alpha\beta}_{ij} \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}_j} c_{\mathbf{q}\beta}$$

$$= \sum_{\mathbf{k}}\sum_{\alpha\beta}\sum_{\mathbf{q}} c^\dagger_{\mathbf{k}\alpha}\left(\frac{1}{N}\sum_{ij} e^{i(\mathbf{q}\cdot\mathbf{r}_j - \mathbf{k}\cdot\mathbf{r}_i)} h^{\alpha\beta}_{i-j}\right) c_{\mathbf{q}\beta}$$

$$= \sum_{\mathbf{k}}\sum_{\alpha\beta}\sum_{\mathbf{q}} c^\dagger_{\mathbf{k}\alpha}\left(\frac{1}{N}\sum_{\mathbf{R}\mathbf{r}} e^{i(\mathbf{q}-\mathbf{k})\cdot\mathbf{R}} e^{-i(\mathbf{q}+\mathbf{k})\cdot\mathbf{r}/2} h^{\alpha\beta}_{\mathbf{r}}\right) c_{\mathbf{q}\beta} \quad (\mathbf{r}_i = \mathbf{R} + \frac{\mathbf{r}}{2},\ \mathbf{r}_j = \mathbf{R} - \frac{\mathbf{r}}{2})$$

$$= \sum_{\mathbf{k}}\sum_{\alpha\beta}\sum_{\mathbf{q}} c^\dagger_{\mathbf{k}\alpha}\left(\delta_{\mathbf{k}\mathbf{q}}\sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} h^{\alpha\beta}_{\mathbf{r}}\right) c_{\mathbf{q}\beta} \quad (\because \frac{1}{N}\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} = \delta_{\mathbf{k},0})$$

$$= \sum_{\mathbf{k}}\sum_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha} \underbrace{\left(\sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} h^{\alpha\beta}_{\mathbf{r}}\right)}_{= h^{\alpha\beta}_{\mathbf{k}}} c_{\mathbf{k}\beta}$$

Current Operator in Tight-Binding Model (cont.)

- density operator in tight-binding model

$$\rho_i(t) = \sum_\alpha c_{i\alpha}^\dagger c_{i\alpha} \quad \to \quad \rho_{\mathbf{q}}(t) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}\alpha} \tag{44}$$

TI-16: proof of Eq. (44)

- current operator from the continuity equation

$$\mathbf{q} \cdot \mathbf{j}_{\mathbf{q}} = -\frac{1}{\hbar} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \sum_{\alpha\beta} (h_{\mathbf{k}-\mathbf{q}/2}^{\alpha\beta} - h_{\mathbf{k}+\mathbf{q}/2}^{\alpha\beta}) c_{\mathbf{k}-\mathbf{q}/2\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}/2\beta} \tag{45}$$

TI-17: proof of Eq. (45)

- small q limit
  - low-energy and long-wavelength fields are more relevant in practical experiment
  - this approximation is valid as long as the field variation is larger than several lattice spacings

Current Operator in Tight-Binding Model (cont.)

TI-16: proof of Eq. (44)

The Fourier transform of the density operator is (omitting the summation over the orbital indices)

$$\begin{aligned}
\rho_{\mathbf{q}} &= \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i} c_{i\alpha}^\dagger c_{i\alpha} \\
&= \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\alpha}^\dagger \frac{1}{\sqrt{N}} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}_i} c_{\mathbf{p}\alpha} \\
&= \frac{1}{\sqrt{N}} \sum_{\mathbf{kp}} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{p}\alpha} \frac{1}{N} \sum_i e^{i(\mathbf{p}-\mathbf{k}-\mathbf{q})\cdot\mathbf{r}_i} \\
&= \frac{1}{\sqrt{N}} \sum_{\mathbf{kp}} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{p}\alpha} \delta_{\mathbf{p},\mathbf{k}+\mathbf{q}} \\
&= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}\alpha}
\end{aligned}$$

Current Operator in Tight-Binding Model (cont.)

TI-17: proof of Eq. (45)

The current satisfies

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r}, t) = 0.$$

By expressing the density and current in terms of their Fourier components,

$$0 = \frac{\partial}{\partial t} \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \rho_{\mathbf{q}} + \boldsymbol{\nabla} \cdot \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \mathbf{j}_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \left(\frac{\partial \rho_{\mathbf{q}}}{\partial t} + i\mathbf{q} \cdot \mathbf{j}_{\mathbf{q}} \right) \quad \rightarrow \quad \mathbf{q} \cdot \mathbf{j}_{\mathbf{q}} = i \frac{\partial \rho_{\mathbf{q}}}{\partial t}$$

Now we compute the time derivative of the density operator

$$\frac{\partial \rho_{\mathbf{q}}}{\partial t} = \frac{i}{\hbar} [\mathcal{H}, \rho_{\mathbf{q}}] = \frac{i}{\hbar} [\sum_{\mathbf{k}} \sum_{\alpha\beta} c^{\dagger}_{\mathbf{k}\alpha} h^{\alpha\beta}_{\mathbf{k}} c_{\mathbf{k}\beta}, \frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} \sum_{\alpha'} c^{\dagger}_{\mathbf{k}'\alpha'} c_{\mathbf{k}'+\mathbf{q}\alpha'}]$$

Using $[c_1^\dagger c_2, c_3^\dagger c_4] = c_1^\dagger [c_2, c_3^\dagger c_4] + [c_1^\dagger, c_3^\dagger c_4] c_2 = c_1^\dagger \{c_2, c_3^\dagger\} c_4 - c_3^\dagger \{c_1^\dagger, c_4\} c_2 = \delta_{23} c_1^\dagger c_4 - \delta_{14} c_3^\dagger c_2$, one obtains

$$\frac{\partial \rho_{\mathbf{q}}}{\partial t} = \frac{1}{\sqrt{N}} \frac{i}{\hbar} \sum_{\mathbf{k}\mathbf{k}'} \sum_{\alpha\beta\alpha'} h^{\alpha\beta}_{\mathbf{k}} \left(\delta_{\mathbf{k},\mathbf{k}'} \delta_{\beta\alpha'} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}'+\mathbf{q}\alpha'} - \delta_{\mathbf{k},\mathbf{k}'+\mathbf{q}} \delta_{\alpha\alpha'} c^{\dagger}_{\mathbf{k}'\alpha'} c_{\mathbf{k}\beta} \right)$$

$$= \frac{1}{\sqrt{N}} \frac{i}{\hbar} \sum_{\mathbf{k}} \sum_{\alpha\beta} h^{\alpha\beta}_{\mathbf{k}} \left(c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}+\mathbf{q}\beta} - c^{\dagger}_{\mathbf{k}-\mathbf{q}\alpha} c_{\mathbf{k}\beta} \right)$$

$$= \frac{1}{\sqrt{N}} \frac{i}{\hbar} \sum_{\mathbf{k}} \sum_{\alpha\beta} (h^{\alpha\beta}_{\mathbf{k}} - h^{\alpha\beta}_{\mathbf{k}+\mathbf{q}}) c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}+\mathbf{q}\beta}$$

Current Operator in Tight-Binding Model (cont.)

Therefore,

$$\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}} = -\frac{1}{\hbar}\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\alpha\beta}(h_{\mathbf{k}}^{\alpha\beta} - h_{\mathbf{k}+\mathbf{q}}^{\alpha\beta})c_{\mathbf{k}\alpha}^{\dagger}c_{\mathbf{k}+\mathbf{q}\beta} = -\frac{1}{\hbar}\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\alpha\beta}(h_{\mathbf{k}-\mathbf{q}/2}^{\alpha\beta} - h_{\mathbf{k}+\mathbf{q}/2}^{\alpha\beta})c_{\mathbf{k}-\mathbf{q}/2\alpha}^{\dagger}c_{\mathbf{k}+\mathbf{q}/2\beta}$$

where in the last step we have shifted $\mathbf{k} \to \mathbf{k} - \mathbf{q}/2$.

Current Operator in Tight-Binding Model (cont.)

- current operator in small q limit

$$\mathbf{j}_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\alpha\beta} \frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial \hbar \mathbf{k}} c_{\mathbf{k}-\mathbf{q}/2\alpha}^{\dagger} c_{\mathbf{k}+\mathbf{q}/2\beta} \tag{46}$$

TI-18: proof of Eq. (46)

Current Operator in Tight-Binding Model (cont.)

TI-18: proof of Eq. (46)

By expanding with respect to $\mathbf{q}$,

$$h^{\alpha\beta}_{\mathbf{k}-\mathbf{q}/2} - h^{\alpha\beta}_{\mathbf{k}+\mathbf{q}/2} = \sum_{n=0}^{\infty} \frac{1}{n!}\left[\left(-\frac{\mathbf{q}}{2}\cdot\boldsymbol{\nabla}_{\mathbf{k}}\right)^n h^{\alpha\beta}_{\mathbf{k}} - \left(\frac{\mathbf{q}}{2}\cdot\boldsymbol{\nabla}_{\mathbf{k}}\right)^n h^{\alpha\beta}_{\mathbf{k}}\right]$$
$$= -\frac{\partial h^{\alpha\beta}_{\mathbf{k}}}{\partial \mathbf{k}}\cdot\mathbf{q} + \mathcal{O}(q^3)$$

Note that no even-power terms remain. Therefore,

$$\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\sum_{\alpha\beta}\frac{1}{\hbar}\mathbf{q}\cdot\frac{\partial h^{\alpha\beta}_{\mathbf{k}}}{\partial \mathbf{k}} c^{\dagger}_{\mathbf{k}-\mathbf{q}/2\alpha} c_{\mathbf{k}+\mathbf{q}/2\beta} + \mathcal{O}(q^3)$$

Current Operator in Tight-Binding Model (cont.)

- Peierls substitution: minimal coupling of the vector potential in the tight-binding model
  - $h_{ij}^{\alpha\beta}$: hopping strength coming from overlap integrals between the atomic orbitals of neighboring atoms
  - in the presence of electromagnetic field, $\mathbf{p} \to \mathbf{p} - \frac{e}{c}\mathbf{A}$ in the continuum Hamiltonian
  - the minimal coupling changes the phase of every hopping matrix element in the following way

$$h_{ij}^{\alpha\beta} \to h_{ij}^{\alpha\beta} \exp\left[\frac{ie}{\hbar c}\int_{\mathbf{r}_i}^{\mathbf{r}_j} d\mathbf{r}\cdot\mathbf{A}(\mathbf{r})\right] \tag{47}$$

  - taking the shortest path, that is, a straight line connecting two sites and assuming that the vector potential does not vary wildly over a few lattice sites

$$\int_{\mathbf{r}_i}^{\mathbf{r}_j} d\mathbf{r}\cdot\mathbf{A}(\mathbf{r}) \approx (\mathbf{r}_j - \mathbf{r}_i)\cdot\mathbf{A}(\frac{\mathbf{r}_i+\mathbf{r}_j}{2}, t) \tag{48}$$

TI-19: proof of Eq. (47)

Current Operator in Tight-Binding Model (cont.)

TI-19: proof of Eq. (47)

First, we consider the continuum model with the Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2 + \cdots = \frac{1}{2m}\left(i\hbar\boldsymbol{\nabla} + \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2 + \cdots$$

Now we introduce a gauge transformation for wavefunction $\psi(\mathbf{r})$:

$$\psi(\mathbf{r}) = \psi'(\mathbf{r})\exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}} d\mathbf{r}'\cdot\mathbf{A}(\mathbf{r}')\right]$$

Since

$$\begin{aligned}\left(i\hbar\boldsymbol{\nabla} + \frac{e}{c}\mathbf{A}\right)\exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}} d\mathbf{r}'\cdot\mathbf{A}(\mathbf{r}')\right]\psi'(\mathbf{r}) &= \exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}} d\mathbf{r}'\cdot\mathbf{A}(\mathbf{r}')\right]\left(i\hbar\boldsymbol{\nabla} + (i\hbar)\times\frac{i}{\hbar}\frac{e}{c}\mathbf{A} + \frac{e}{c}\mathbf{A}\right)\psi'(\mathbf{r}) \\ &= \exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}} d\mathbf{r}'\cdot\mathbf{A}(\mathbf{r}')\right] i\hbar\boldsymbol{\nabla}\psi'(\mathbf{r})\end{aligned}$$

one obtains

$$\begin{aligned}H\psi(\mathbf{r}) &= \left[\frac{1}{2m}\left(i\hbar\boldsymbol{\nabla} + \frac{e}{c}\mathbf{A}\right)^2 + \cdots\right]\psi(\mathbf{r}) \\ &= \exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}} d\mathbf{r}'\cdot\mathbf{A}(\mathbf{r}')\right]\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \cdots\right]\psi'(\mathbf{r})\end{aligned}$$

It implies that the effect of the vector potential can be moved into the additional phase of the wave function. After the gauge transformation, the Hamiltonian turns back to that ($\mathcal{H}_0$) without the field.

Current Operator in Tight-Binding Model (cont.)

Now we discretize the operators in order to construct the tight-binding Hamiltonian:

$$\begin{aligned}\mathcal{H}\psi_i &= \exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}_i} d\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right]\mathcal{H}_0\psi_i' \\ &= \exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}_i} d\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right]\sum_j h_{ij}^{(0)}\psi_j' \\ &= \exp\left[\frac{ie}{\hbar c}\int^{\mathbf{r}_i} d\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right]\sum_j h_{ij}^{(0)}\exp\left[-\frac{ie}{\hbar c}\int^{\mathbf{r}_j} d\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right]\psi_j \\ &= \sum_j h_{ij}\psi_j\end{aligned}$$

where

$$h_{ij} = h_{ij}^{(0)}\exp\left[\frac{ie}{\hbar c}\int_{\mathbf{r}_j}^{\mathbf{r}_i} d\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right]$$

Current Operator in Tight-Binding Model (cont.)

- weak electromagnetic field: up to the linear order in $\mathbf{A}(\mathbf{r}, t)$
  - second order $\rightarrow A^2$-term (diamagnetic term)
  - the contribution from the diamagnetic term is diagonal in the spatial indices, which is irrelevant to the Hall conductance

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{ext}} \tag{49}$$

with

$$\mathcal{H}_{\text{ext}} = -\frac{e}{c} \sum_{\mathbf{q}} \mathbf{j}_{-\mathbf{q}} \cdot \mathbf{A}_{\mathbf{q}}(t) \tag{50}$$

Note that this expression is same as that for the continuum model, Eq. (39).

TI-20: proof of Eq. (49)

Current Operator in Tight-Binding Model (cont.)

TI-20: proof of Eq. (49)

Up to the linear order in $\mathbf{A}(\mathbf{r}, t)$,

$$h_{ij}^{\alpha\beta} \to h_{ij}^{\alpha\beta} \exp\left[\frac{ie}{\hbar c}\int_{\mathbf{r}_j}^{\mathbf{r}_i} d\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right] \approx h_{ij}^{\alpha\beta}\left(1 + \frac{ie}{\hbar c}\int_{\mathbf{r}_j}^{\mathbf{r}_i} d\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')\right)$$
$$= h_{ij}^{\alpha\beta}\left(1 + \frac{ie}{\hbar c}\mathbf{A}(\frac{\mathbf{r}_i + \mathbf{r}_j}{2}, t) \cdot (\mathbf{r}_i - \mathbf{r}_j)\right)$$

Then, the Hamiltonian change due to the field is then

$$\mathcal{H}_{\text{ext}} = \sum_{ij}\sum_{\alpha\beta} c_{i\alpha}^\dagger h_{ij}^{\alpha\beta} \frac{ie}{\hbar c}\mathbf{A}(\frac{\mathbf{r}_i + \mathbf{r}_j}{2}, t) \cdot (\mathbf{r}_i - \mathbf{r}_j) c_{j\beta}$$

Noting the translational invariance of the Hamiltonian, we have $h_{ij} = h_{i-j} = h_{\mathbf{r}}$ and $\mathbf{r}_i - \mathbf{r}_j = \mathbf{r}$. So,

$$\mathcal{H}_{\text{ext}} = \sum_{ij}\sum_{\alpha\beta}\left(\frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\alpha}^\dagger\right) h_{i-j}^{\alpha\beta}\frac{ie}{\hbar c}\mathbf{A}(\frac{\mathbf{r}_i + \mathbf{r}_j}{2}, t) \cdot (\mathbf{r}_i - \mathbf{r}_j)\left(\frac{1}{\sqrt{N}}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}_j} c_{\mathbf{p}\beta}\right)$$
$$= \sum_{\mathbf{kp}}\sum_{\alpha\beta} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{p}\beta}\frac{1}{N}\sum_{j,\mathbf{r}} e^{i\mathbf{p}\cdot\mathbf{r}_j} e^{-i\mathbf{k}\cdot(\mathbf{r}_j+\mathbf{r})} h_{\mathbf{r}}^{\alpha\beta}\frac{ie}{\hbar c}\mathbf{A}(\mathbf{r}_j + \frac{\mathbf{r}}{2}, t) \cdot \mathbf{r}$$
$$= \sum_{\mathbf{kp}}\sum_{\alpha\beta} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{p}\beta}\frac{1}{N}\sum_{j,\mathbf{r}} e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{r}_j} e^{-i\mathbf{k}\cdot\mathbf{r}} h_{\mathbf{r}}^{\alpha\beta}\frac{ie}{\hbar c}\frac{1}{\sqrt{N}}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{r}_j+\mathbf{r}/2)}\mathbf{A}_{\mathbf{q}}(t) \cdot \mathbf{r}$$
$$= \frac{e}{c}\sum_{\mathbf{kpq}}\sum_{\alpha\beta} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{p}\beta}\underbrace{\left(\frac{1}{N}\sum_{j} e^{i(\mathbf{p}-\mathbf{k}+\mathbf{q})\cdot\mathbf{r}_j}\right)}_{=\delta_{\mathbf{p},\mathbf{k}-\mathbf{q}}}\left(\frac{1}{\hbar}\frac{1}{\sqrt{N}}\sum_{\mathbf{r}} i\mathbf{r} e^{i(\mathbf{q}/2-\mathbf{k})\cdot\mathbf{r}} h_{\mathbf{r}}^{\alpha\beta}\right) \cdot \mathbf{A}_{\mathbf{q}}(t)$$

Current Operator in Tight-Binding Model (cont.)

$$= \frac{e}{c} \sum_{\mathbf{kq}} \sum_{\alpha\beta} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}-\mathbf{q}\beta} \left(\frac{1}{\hbar} \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} i\mathbf{r} e^{i(\mathbf{q}/2-\mathbf{k})\cdot\mathbf{r}} h^{\alpha\beta}_{\mathbf{r}} \right) \cdot \mathbf{A}_{\mathbf{q}}(t)$$

By shifting $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{q}/2$,

$$\mathcal{H}_{\text{ext}} = -\frac{e}{c} \frac{1}{\sqrt{N}} \sum_{\mathbf{kq}} \sum_{\alpha\beta} c^{\dagger}_{\mathbf{k}+\mathbf{q}/2\alpha} c_{\mathbf{k}-\mathbf{q}/2\beta} \underbrace{\left(\frac{1}{\hbar} \sum_{\mathbf{r}} (-i\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} h^{\alpha\beta}_{\mathbf{r}} \right)}_{= \frac{\partial h^{\alpha\beta}_{\mathbf{k}}}{\partial \hbar \mathbf{k}}} \cdot \mathbf{A}_{\mathbf{q}}(t)$$

$$= -\frac{e}{c} \sum_{\mathbf{q}} \left(\frac{1}{\sqrt{N}} \sum_{\mathbf{k}\alpha\beta} \frac{\partial h^{\alpha\beta}_{\mathbf{k}}}{\partial \hbar \mathbf{k}} c^{\dagger}_{\mathbf{k}+\mathbf{q}/2\alpha} c_{\mathbf{k}-\mathbf{q}/2\beta} \right) \cdot \mathbf{A}_{\mathbf{q}}(t)$$

$$= -\frac{e}{c} \sum_{\mathbf{q}} \mathbf{j}_{-\mathbf{q}} \cdot \mathbf{A}_{\mathbf{q}}(t)$$

Outline

Linear Response Theory

- setup for linear response theory

$$\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_{\text{ext}}(t) \tag{51}$$

  - unperturbed Hamiltonian $\mathcal{H}_0$
  - weak time-dependent perturbation $\mathcal{H}_{\text{ext}}(t)$ turned on at $t = t_0$
  - the perturbation is weak enough that the system is still in (local) equilibrium $\rightarrow$ equilibrium statistical mechanics
    $\rightarrow$ density matrix operator

$$\rho(t) = \frac{1}{\mathcal{Z}} e^{-\beta(\mathcal{H}(t) - \mu\mathcal{N})} \tag{52}$$

here we set $\mu = 0$.

Linear Response Theory (cont.)

- perturbation to density matrix due to $\mathcal{H}_{\rm ext}$, up to the linear order in $\mathcal{H}_{\rm ext}$,

$$\rho(t) = \rho_0 + \delta\rho(t) \tag{53}$$

where ρ_0 is the unperturbed density matrix when $\mathcal{H} = \mathcal{H}_0$. In the interaction picture with respect to $\mathcal{H}$ or in the Heisenberg picture with respect to $\mathcal{H}_0$,

$$\delta\rho(t) = \frac{i}{\hbar}\int_{t_0}^{t} dt' [\rho_0, \mathcal{H}_{{\rm ext},I}(t'-t)] \tag{54}$$

TI-21: proof of Eq. (54)

- change in $\langle \mathcal{B}(t) \rangle$ due to the perturbation

$$\delta \langle \mathcal{B}(t) \rangle = \frac{i}{\hbar}\int_{t_0}^{t} dt' \, \langle [\mathcal{H}_{\rm ext}(t'), \mathcal{B}(t)] \rangle_0 \tag{55}$$

where the Heisenberg picture with respect to the unperturbed Hamiltonian $\mathcal{H}_0$ is used.

TI-22: proof of Eq. (55)

Linear Response Theory (cont.)

TI-21: proof of Eq. (54)

Here we use the interaction picture:

$$\rho_I(t) = e^{\frac{i}{\hbar}\mathcal{H}_0 t}\rho(t)e^{-\frac{i}{\hbar}\mathcal{H}_0 t}$$

(compare to the Heisenberg picture, $O_H(t) = e^{\frac{i}{\hbar}\mathcal{H}t}Oe^{-\frac{i}{\hbar}\mathcal{H}t}$). From the von Neumann equation,

$$\frac{\partial\rho(t)}{\partial t} = -\frac{i}{\hbar}[\mathcal{H}, \rho(t)].$$

Then, the time derivative of the density matrix in the interaction picture is given by

$$\begin{aligned}\frac{\partial\rho_I(t)}{\partial t} &= \frac{i}{\hbar}\left(e^{\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{H}_0\rho(t)e^{-\frac{i}{\hbar}\mathcal{H}_0 t} - e^{\frac{i}{\hbar}\mathcal{H}_0 t}\rho(t)\mathcal{H}_0 e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\right) + e^{\frac{i}{\hbar}\mathcal{H}_0 t}\frac{\partial\rho(t)}{\partial t}e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\\ &= \frac{i}{\hbar}e^{\frac{i}{\hbar}\mathcal{H}_0 t}[\mathcal{H}_0, \rho(t)]e^{-\frac{i}{\hbar}\mathcal{H}_0 t} - \frac{i}{\hbar}e^{\frac{i}{\hbar}\mathcal{H}_0 t}[\mathcal{H}(t), \rho(t)]e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\\ &= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\mathcal{H}_0 t}[\mathcal{H}_{\text{ext}}(t), \rho(t)]e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\end{aligned}$$

Since

$$\frac{\partial\rho_0}{\partial t} = -\frac{i}{\hbar}[\mathcal{H}_0, \rho_0] = 0 = \frac{\partial\rho_{0,I}}{\partial t},$$

the time derivative of the perturbation $\delta\rho(t)$ is, up to the linear order in $\mathcal{H}_{\text{ext}}$,

$$\begin{aligned}\frac{\partial\delta\rho_I(t)}{\partial t} = \frac{\partial\rho_I(t)}{\partial t} &= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\mathcal{H}_0 t}[\mathcal{H}_{\text{ext}}(t), \rho_0 + \delta\rho(t)]e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\\ &= -\frac{i}{\hbar}e^{\frac{i}{\hbar}\mathcal{H}_0 t}[\mathcal{H}_{\text{ext}}(t), \rho_0]e^{-\frac{i}{\hbar}\mathcal{H}_0 t} - \frac{i}{\hbar}e^{\frac{i}{\hbar}\mathcal{H}_0 t}\underbrace{[\mathcal{H}_{\text{ext}}(t), \delta\rho(t)]}_{\sim\mathcal{O}(\mathcal{H}_{\text{ext}}^2)}e^{-\frac{i}{\hbar}\mathcal{H}_0 t} \approx -\frac{i}{\hbar}[\mathcal{H}_{\text{ext},I}(t), \rho_0]\end{aligned}$$

Linear Response Theory (cont.)

By integrating over time and using the fact that $\mathcal{H}_{\text{ext}}$ is turned on at $t = t_0$,

$$\delta\rho_I(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt' [\mathcal{H}_{\text{ext},I}(t'), \rho_0]$$

or

$$\begin{aligned}
\delta\rho(t) &= e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\delta\rho_I(t)e^{\frac{i}{\hbar}\mathcal{H}_0 t} = -\frac{i}{\hbar}\int_{t_0}^{t} dt' e^{-\frac{i}{\hbar}\mathcal{H}_0 t}[\mathcal{H}_{\text{ext},I}(t'), \rho_0]e^{\frac{i}{\hbar}\mathcal{H}_0 t} \\
&= \frac{i}{\hbar}\int_{t_0}^{t} dt' [\rho_0, e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{H}_{\text{ext},I}(t')e^{\frac{i}{\hbar}\mathcal{H}_0 t}] \\
&= \frac{i}{\hbar}\int_{t_0}^{t} dt' [\rho_0, \mathcal{H}_{\text{ext},I}(t' - t)]
\end{aligned}$$

where we have used

$$\begin{aligned}
e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{H}_{\text{ext},I}(t')e^{\frac{i}{\hbar}\mathcal{H}_0 t} &= e^{-\frac{i}{\hbar}\mathcal{H}_0 t}e^{\frac{i}{\hbar}\mathcal{H}_0 t'}\mathcal{H}_{\text{ext}}e^{-\frac{i}{\hbar}\mathcal{H}_0 t'}e^{\frac{i}{\hbar}\mathcal{H}_0 t} \\
&= e^{\frac{i}{\hbar}\mathcal{H}_0(t'-t)}\mathcal{H}_{\text{ext}}e^{-\frac{i}{\hbar}\mathcal{H}_0(t'-t)} \\
&= \mathcal{H}_{\text{ext},I}(t' - t)
\end{aligned}$$

Linear Response Theory (cont.)

TI-22: proof of Eq. (55)

Let $\delta\langle\mathcal{B}(t)\rangle \equiv \langle\mathcal{B}(t)\rangle - \langle\mathcal{B}\rangle_0$, where $\langle\mathcal{B}(t)\rangle = \mathrm{Tr}[\rho(t)\mathcal{B}]$ and $\langle\mathcal{B}\rangle_0 = \mathrm{Tr}[\rho_0\mathcal{B}]$. Then,

$$\begin{aligned}\delta\langle\mathcal{B}(t)\rangle &= \langle\mathcal{B}(t)\rangle - \langle\mathcal{B}\rangle_0 = \mathrm{Tr}[(\rho(t)-\rho_0)\mathcal{B}] = \mathrm{Tr}[\delta\rho(t)\mathcal{B}] \\ &= \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\mathrm{Tr}\left\{[\rho_0, \mathcal{H}_{\mathrm{ext},I}(t'-t)]\mathcal{B}\right\}\end{aligned}$$

Using

$$\mathrm{Tr}\{[\mathcal{A},\mathcal{B}]\mathcal{C}\} = \mathrm{Tr}[\mathcal{ABC} - \mathcal{BAC}] = \mathrm{Tr}[\mathcal{ABC} - \mathcal{ACB}] = \mathrm{Tr}\{\mathcal{A}[\mathcal{B},\mathcal{C}]\}$$

one obtains (using the fact ρ_0 and $\mathcal{H}_0$ commute with each other and $\mathrm{Tr}[\mathcal{AB}] = \mathrm{Tr}[\mathcal{BA}]$)

$$\begin{aligned}\mathrm{Tr}\left\{[\rho_0, \mathcal{H}_{\mathrm{ext},I}(t'-t)]\mathcal{B}\right\} &= \mathrm{Tr}\left\{\rho_0[\mathcal{H}_{\mathrm{ext},I}(t'-t), \mathcal{B}]\right\} \\ &= \mathrm{Tr}\left\{\rho_0[e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{H}_{\mathrm{ext},I}(t')e^{\frac{i}{\hbar}\mathcal{H}_0 t}, \mathcal{B}]\right\} \\ &= \mathrm{Tr}\left\{\rho_0\left(e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{H}_{\mathrm{ext},I}(t')e^{\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{B} - \mathcal{B}e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{H}_{\mathrm{ext},I}(t')e^{\frac{i}{\hbar}\mathcal{H}_0 t}\right)\right\} \\ &= \mathrm{Tr}\left\{\rho_0\left(\mathcal{H}_{\mathrm{ext},I}(t')e^{\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{B}e^{-\frac{i}{\hbar}\mathcal{H}_0 t} - e^{\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{B}e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{H}_{\mathrm{ext},I}(t')\right)\right\} \\ &= \mathrm{Tr}\left\{\rho_0[\mathcal{H}_{\mathrm{ext},I}(t'), \mathcal{B}_I(t)]\right\}\end{aligned}$$

Now we returns back to the Heisenberg picture with respect to $\mathcal{H}_0$. Then, $\mathcal{A}_I(t) = \mathcal{A}_H(t) = \mathcal{A}(t)$, so

$$\delta\langle\mathcal{B}(t)\rangle = \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\mathrm{Tr}\left\{\rho_0[\mathcal{H}_{\mathrm{ext}}(t'), \mathcal{B}(t)]\right\} = \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\langle[\mathcal{H}_{\mathrm{ext}}(t'), \mathcal{B}(t)]\rangle_0$$

where the subscript 0 means that the expectation value is calculated with respect to the density matrix for the unperturbed Hamiltonian $\mathcal{H}_0$.

Linear Response Theory (cont.)

- linear response and retarded Green's function: suppose that the perturbation is coupled to the system by the operator $\mathcal{A}^\dagger(t)$
  - for $\mathcal{H}_{\mathrm{ext}}(t) = \mathcal{A}^\dagger(t)h(t)$,

$$\delta\langle\mathcal{B}(t)\rangle = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt'\, \mathcal{G}^R_{\mathcal{B}\mathcal{A}}(t,t')h(t') \tag{56}$$

  where $\mathcal{G}^R_{\mathcal{B}\mathcal{A}}$ is the retarded Green's function defined by

$$\mathcal{G}^R_{\mathcal{B}\mathcal{A}}(t,t') \equiv -i\Theta(t-t')\left\langle[\mathcal{B}(t),\mathcal{A}^\dagger(t')]\right\rangle_0 . \tag{57}$$

  - for $\mathcal{H}_{\mathrm{ext}}(t) = \int d^3r\, \mathcal{A}^\dagger(\mathbf{r},t)h(\mathbf{r},t)$,

$$\delta\langle\mathcal{B}(\mathbf{r},t)\rangle = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt' \int d^3r'\, \mathcal{G}^R_{\mathcal{B}\mathcal{A}}(\mathbf{r}t,\mathbf{r}'t')h(\mathbf{r}',t') \tag{58}$$

  with

$$\mathcal{G}^R_{\mathcal{B}\mathcal{A}}(\mathbf{r}t,\mathbf{r}'t') \equiv -i\Theta(t-t')\left\langle[\mathcal{B}(\mathbf{r},t),\mathcal{A}^\dagger(\mathbf{r}',t')]\right\rangle_0 . \tag{59}$$

TI-23: proof of Eq. (56)

Linear Response Theory (cont.)

TI-23: proof of Eq. (56)

Since $\mathcal{H}_{\rm ext}(t) = \mathcal{A}^\dagger(t)h(t)$,

$$\delta\langle\mathcal{B}(t)\rangle = \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \langle[\mathcal{H}_{\rm ext}(t'), \mathcal{B}(t)]\rangle_0 = \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \langle[\mathcal{A}^\dagger(t')h(t'), \mathcal{B}(t)]\rangle_0$$

By taking the limit $t_0 \to -\infty$,

$$\begin{aligned}\delta\langle\mathcal{B}(t)\rangle &= -\frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \langle[\mathcal{B}(t), \mathcal{A}^\dagger(t')]\rangle_0\, h(t') = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt'\,\Theta(t-t')\left(-i\langle[\mathcal{B}(t), \mathcal{A}^\dagger(t')]\rangle_0\right) h(t') \\ &= \frac{1}{\hbar}\int_{-\infty}^{\infty} dt'\, \underbrace{\left(-i\Theta(t-t')\langle[\mathcal{B}(t), \mathcal{A}^\dagger(t')]\rangle_0\right)}_{=\mathcal{G}^R_{\mathcal{B}\mathcal{A}}(t,t')} h(t')\end{aligned}$$

Current-current Correlation Function

- perturbation due to weak electromagnetic field

$$\mathcal{H}_{\text{ext}} = -\frac{e}{c}\int d^3r\,\mathbf{A}(\mathbf{r},t)\cdot\mathbf{j}(\mathbf{r},t) = -\frac{e}{c}\sum_{\mathbf{q}}\mathbf{A}_{\mathbf{q}}(t)\cdot\mathbf{j}_{-\mathbf{q}} \tag{60}$$

In case of $\mathbf{E}(\mathbf{r},t) = \mathbf{E}e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}$,

$$\mathbf{A}(\mathbf{r},t) = \frac{\mathbf{E}(\mathbf{r},t)}{i\omega} \quad \text{or} \quad \mathbf{A}_{\mathbf{q}'}(t) = \delta_{\mathbf{q}',\mathbf{q}}\frac{\mathbf{E}_{\mathbf{q}}}{i\omega} \tag{61}$$

- current response with respect to the perturbation: with $s, s' = x, y, z$,

$$\langle j_s(\mathbf{r},t)\rangle = -\frac{e}{\hbar c}\int_{-\infty}^{\infty} dt' \int d^3r'\,\mathcal{D}^R_{ss'}(\mathbf{r}-\mathbf{r}', t-t')A_{s'}(\mathbf{r}', t') \tag{62}$$

with the retarded Green's function (or current-current correlation function)

$$\mathcal{D}^R_{ss'}(\mathbf{r}-\mathbf{r}', t-t') = -i\Theta(t)\left\langle [j_s(\mathbf{r},t), j_{s'}(\mathbf{r}',t')]\right\rangle_0 \tag{63}$$

where we have assumed that the system has translational symmetry and $\mathcal{H}_0$ is time-independent so that $\mathcal{D}^R$ depends only on the differences, $\mathbf{r}-\mathbf{r}'$ and $t-t'$.

TI-24: proof of Eq. (62)

Current-current Correlation Function (cont.)

TI-24: proof of Eq. (62)

According to the linear response theory

$$\begin{aligned}\langle j_s(\mathbf{r},t)\rangle &= \frac{1}{\hbar}\int_{-\infty}^{\infty} dt' \int d^3r' \left(-i\Theta(t)\,\langle [j_s(\mathbf{r},t), j_{s'}(\mathbf{r}',t')\,(-\tfrac{e}{c}A_{s'}(\mathbf{r}',t'))]\rangle_0\right)\\ &= -\frac{e}{\hbar c}\int_{-\infty}^{\infty} dt' \int d^3r' \underbrace{\left(-i\Theta(t)\,\langle [j_s(\mathbf{r},t), j_{s'}(\mathbf{r}',t')]\rangle_0\right)}_{=\mathcal{D}^R_{ss'}} A_{s'}(\mathbf{r}',t')\end{aligned}$$

Retarded and Time-Ordered Green's Functions

- for simplicity, time translational symmetry is assumed
- retarded Green's function

$$\mathcal{G}^R(t) = -i\Theta(t)\left\langle[\mathcal{A}(t), \mathcal{B}(0)]_\pm\right\rangle \tag{64}$$

- time-ordered Green's function

$$\mathcal{G}^t(t) = -i\left\langle\mathcal{T}_t\mathcal{A}(t)\mathcal{B}(0)\right\rangle = -i\left[\Theta(t)\left\langle\mathcal{A}(t)\mathcal{B}(0)\right\rangle \mp \Theta(-t)\left\langle\mathcal{B}(0)\mathcal{A}(t)\right\rangle\right] \tag{65}$$

  where the upper/lower sign corresponds to fermionic/bosonic operators
- two correlation functions

$$\begin{aligned} J_1(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\left\langle\mathcal{A}(t)\mathcal{B}(0)\right\rangle = 2\pi\hbar\sum_{nm}\frac{e^{-\beta E_m}}{\mathcal{Z}}\left\langle n|\mathcal{B}|m\right\rangle\left\langle m|\mathcal{A}|n\right\rangle\delta(E_m - E_n + \hbar\omega) \\ J_2(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\left\langle\mathcal{B}(0)\mathcal{A}(t)\right\rangle = 2\pi\hbar\sum_{nm}\frac{e^{-\beta E_n}}{\mathcal{Z}}\left\langle n|\mathcal{B}|m\right\rangle\left\langle m|\mathcal{A}|n\right\rangle\delta(E_m - E_n + \hbar\omega) \\ &= e^{-\beta\hbar\omega}J_1(\omega) \end{aligned} \tag{66}$$

  where $|m\rangle$, $|n\rangle$ are eigenstates of $\mathcal{H}_0$ so that $\mathcal{H}_0|n\rangle = E_n|n\rangle$.

TI-25: proof of Eq. (66)

Retarded and Time-Ordered Green's Functions (cont.)

TI-25: proof of Eq. (66)

Using the completeness $\sum_m |m\rangle\langle m| = 1$

$$
\begin{aligned}
J_1(t) &\equiv \langle \mathcal{A}(t)\mathcal{B}(0)\rangle \\
&= \mathrm{Tr}\left[\frac{e^{-\beta\mathcal{H}_0}}{\mathcal{Z}} e^{\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{A}e^{-\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{B}\right] \\
&= \sum_n \langle n|\mathcal{B}\frac{e^{-\beta\mathcal{H}_0}}{\mathcal{Z}} e^{\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{A}e^{-\frac{i}{\hbar}\mathcal{H}_0 t}|n\rangle \\
&= \sum_{nm} \langle n|\mathcal{B}\frac{e^{-\beta\mathcal{H}_0}}{\mathcal{Z}}|m\rangle\langle m| e^{\frac{i}{\hbar}\mathcal{H}_0 t}\mathcal{A}e^{-\frac{i}{\hbar}\mathcal{H}_0 t}|n\rangle \\
&= \sum_{nm} \langle n|\mathcal{B}|m\rangle \frac{e^{-\beta E_m}}{\mathcal{Z}} e^{\frac{i}{\hbar}(E_m-E_n)t}\langle m|\mathcal{A}|n\rangle
\end{aligned}
$$

Then, the Fourier transform over the time t is

$$
\begin{aligned}
J_1(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t} J_1(t) \\
&= \sum_{nm} \frac{e^{-\beta E_m}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle\langle m|\mathcal{A}|n\rangle \int_{-\infty}^{\infty} dt\, e^{i(\omega+(E_m-E_n)/\hbar)t} \\
&= 2\pi\hbar \sum_{nm} \frac{e^{-\beta E_m}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle\langle m|\mathcal{A}|n\rangle\, \delta(E_m-E_n+\hbar\omega) \quad \left[\because \int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i\omega t} = \delta(\omega)\right]
\end{aligned}
$$

Retarded and Time-Ordered Green's Functions (cont.)

Similarly,

$$\begin{aligned} J_2(t) &\equiv \langle \mathcal{B}(0)\mathcal{A}(t)\rangle \\ &= \sum_{nm} \langle n| \frac{e^{-\beta \mathcal{H}_0}}{\mathcal{Z}} \mathcal{B}|m\rangle \, \langle m| e^{\frac{i}{\hbar}\mathcal{H}_0 t} \mathcal{A} e^{-\frac{i}{\hbar}\mathcal{H}_0 t}|n\rangle \\ &= \sum_{nm} \frac{e^{-\beta E_n}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \, e^{\frac{i}{\hbar}(E_m - E_n)t} \langle m|\mathcal{A}|n\rangle \end{aligned}$$

and

$$\begin{aligned} J_2(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t} J_2(t) \\ &= 2\pi\hbar \sum_{nm} \frac{e^{-\beta E_n}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \, \langle m|\mathcal{A}|n\rangle \, \delta(E_m - E_n + \hbar\omega) \\ &= 2\pi\hbar \sum_{nm} \frac{e^{-\beta (E_m + \hbar\omega)}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \, \langle m|\mathcal{A}|n\rangle \, \delta(E_m - E_n + \hbar\omega) \\ &= e^{-\beta\hbar\omega} J_1(\omega) \end{aligned}$$

Retarded and Time-Ordered Green's Functions (cont.)

- at zero temperature, $e^{-\beta E_m}/\mathcal{Z} = \delta_{m,0}$ where E_0 is the ground-state energy

$$\begin{aligned} J_1(\omega) &= 2\pi\hbar \sum_m \langle m|\mathcal{B}|0\rangle \langle 0|\mathcal{A}|m\rangle \,\delta(E_0 - E_m + \hbar\omega) \quad \rightarrow \quad J_1(\omega < 0) = 0 \\ J_2(\omega) &= 2\pi\hbar \sum_m \langle 0|\mathcal{B}|m\rangle \langle m|\mathcal{A}|0\rangle \,\delta(E_m - E_0 + \hbar\omega) \quad \rightarrow \quad J_2(\omega > 0) = 0 \end{aligned} \tag{67}$$

- $\mathcal{B} = \mathcal{A}^\dagger \rightarrow J_{1/2}(\omega)$ are real: since $\langle n|\mathcal{B}|m\rangle = \langle n|\mathcal{A}^\dagger|m\rangle = \langle m|\mathcal{A}|n\rangle^*$,

$$J_1(\omega) = 2\pi\hbar \sum_{nm} \frac{e^{-\beta E_m}}{\mathcal{Z}} \left|\langle m|\mathcal{A}|n\rangle\right|^2 \delta(E_m - E_n + \hbar\omega) \tag{68}$$

- $\mathcal{G}^R(\omega)$ and $\mathcal{G}^t(\omega)$ in terms of $J_1(\omega)$

$$\begin{aligned} \mathcal{G}^R(\omega) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{1 \pm e^{-\beta\hbar\omega'}}{\omega - \omega' + i\eta} J_1(\omega') \qquad \text{with} \;\; \eta = 0^+ \\ \mathcal{G}^t(\omega) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left(\frac{1}{\omega - \omega' + i\eta} \pm \frac{e^{-\beta\hbar\omega'}}{\omega - \omega' - i\eta} \right) J_1(\omega') \end{aligned} \tag{69}$$

TI-26: proof of Eq. (69)

Retarded and Time-Ordered Green's Functions (cont.)

TI-26: proof of Eq. (69)

$$\mathcal{G}^R(t) = -i\Theta(t)(J_1(t) - J_2(t))$$
$$\mathcal{G}^t(t) = -i\left[\Theta(t)J_1(t) + \Theta(-t)J_2(t)\right]$$

Using

$$\Theta(t) = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\frac{e^{-i\omega t}}{\omega + i\eta}$$

one can Fourier transform the Green's function as

$$\mathcal{G}^R(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\mathcal{G}^R(t) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\left(\int_{-\infty}^{\infty}\frac{d\omega''}{2\pi}\frac{e^{-i\omega'' t}}{\omega'' + i\eta}\right)\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}e^{-i\omega' t}\left(J_1(\omega') \pm J_2(\omega')\right)$$
$$= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\int_{-\infty}^{\infty} d\omega''\frac{1 \pm e^{-\beta\hbar\omega'}}{\omega'' + i\eta}J_1(\omega')\underbrace{\int_{-\infty}^{\infty}\frac{dt}{2\pi}e^{i(\omega-\omega'-\omega'')t}}_{=\delta(\omega-\omega'-\omega'')}$$
$$= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{1 \pm e^{-\beta\hbar\omega'}}{\omega - \omega' + i\eta}J_1(\omega')$$

Retarded and Time-Ordered Green's Functions (cont.)

Similarly,

$$\begin{aligned}
\mathcal{G}^t(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\mathcal{G}^t(t) \\
&= \int_{-\infty}^{\infty} dt\, e^{i\omega t} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{-i\omega' t} \left[\left(\int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \frac{e^{-i\omega'' t}}{\omega'' + i\eta} \right) J_1(\omega') \mp \left(\int_{-\infty}^{\infty} \frac{d\omega''}{2\pi} \frac{e^{i\omega'' t}}{\omega'' + i\eta} \right) J_2(\omega') \right] \\
&= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} d\omega'' \left[\frac{1}{\omega'' + i\eta} \underbrace{\int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega - \omega' - \omega'')t}}_{= \delta(\omega - \omega' - \omega'')} \mp \frac{e^{-\beta\hbar\omega'}}{\omega'' + i\eta} \underbrace{\int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega - \omega' + \omega'')t}}_{= \delta(\omega - \omega' + \omega'')} \right] J_1(\omega') \\
&= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left(\frac{1}{\omega - \omega' + i\eta} \pm \frac{e^{-\beta\hbar\omega'}}{\omega - \omega' - i\eta} \right) J_1(\omega')
\end{aligned}$$

Retarded and Time-Ordered Green's Functions (cont.)

- relation between $\mathcal{G}^R$ and $\mathcal{G}^t$: when $\mathcal{B} = \mathcal{A}^\dagger$

$$\mathrm{Re}[\mathcal{G}^R(\omega)] = \mathrm{Re}[\mathcal{G}^t(\omega)] = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \mathcal{P} \frac{1 \pm e^{-\beta\hbar\omega'}}{\omega - \omega'} J_1(\omega')$$

$$\mathrm{Im}[\mathcal{G}^R(\omega)] = -\frac{1 \pm e^{-\beta\hbar\omega}}{2} J_1(\omega) \quad \text{and} \quad \mathrm{Im}[\mathcal{G}^t(\omega)] = -\frac{1 \mp e^{-\beta\hbar\omega}}{2} J_1(\omega) \tag{70}$$

$$\rightarrow \quad \mathrm{Im}[\mathcal{G}^R(\omega)] = \left(\tanh \frac{\beta\hbar\omega}{2}\right)^{\mp 1} \mathrm{Im}[\mathcal{G}^t(\omega)]$$

TI-27: proof of Eq. (70)

- fluctuation-dissipation theorem
  - conductivity

$$J_{e,s}(\omega) = \sigma_{ss'}(\omega) E_{s'}(\omega) = \sigma_{ss'}(\omega) i\omega A_{s'}(\omega) \tag{71}$$

  - linear response theory: $J_1(\omega) = \langle j_s(t) j_{s'}(0)\rangle$ and $\mathcal{G}^R(\omega) = \mathcal{D}^R(\omega)$ from Eq. (62). For $s = s'$,

$$i\omega\sigma_{ss}(\omega) = -\frac{e^2}{\hbar c}\mathcal{D}^R_{ss}(\omega) = -\frac{e^2}{\hbar c} i\,\mathrm{Im}[\mathcal{D}^R_{ss}(\omega)] \;\rightarrow\; \sigma_{ss}(\omega) = \frac{e^2}{\hbar c}\frac{1 - e^{-\beta\hbar\omega}}{2} J_1(\omega) \tag{72}$$

which implies that the dissipation ($\sigma(\omega)$) is related to the fluctuation ($J_1(\omega)$).

Retarded and Time-Ordered Green's Functions (cont.)

TI-27: proof of Eq. (70)

Using

$$\frac{1}{\omega \pm i\eta} = \mathcal{P}\frac{1}{\omega} \mp \pi i \delta(\omega)$$

one gets

$$\begin{aligned}
\mathcal{G}^R(\omega) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{1 \pm e^{-\beta\hbar\omega'}}{\omega - \omega' + i\eta} J_1(\omega') \\
&= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left(\mathcal{P}\frac{1 \pm e^{-\beta\hbar\omega'}}{\omega - \omega'} - i\pi(1 \pm e^{-\beta\hbar\omega'})\delta(\omega - \omega') \right) J_1(\omega') \\
&= \underbrace{\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \mathcal{P}\frac{1 \pm e^{-\beta\hbar\omega'}}{\omega - \omega'} J_1(\omega')}_{\text{real part}} + \underbrace{(-i)\frac{1 \pm e^{-\beta\hbar\omega}}{2} J_1(\omega)}_{\text{imaginary part}}
\end{aligned}$$

since $J_1(\omega)$ is real, and

$$\begin{aligned}
\mathcal{G}^t(\omega) &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left(\frac{1}{\omega - \omega' + i\eta} \pm \frac{e^{-\beta\hbar\omega'}}{\omega - \omega' - i\eta} \right) J_1(\omega') \\
&= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \left(\mathcal{P}\frac{1}{\omega - \omega'} - i\pi\delta(\omega - \omega') \pm \mathcal{P}\frac{e^{-\beta\hbar\omega'}}{\omega - \omega'} \pm e^{-\beta\hbar\omega'} i\pi\delta(\omega - \omega') \right) J_1(\omega') \\
&= \underbrace{\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \mathcal{P}\frac{1 \pm e^{-\beta\hbar\omega'}}{\omega - \omega'} J_1(\omega')}_{\text{real part}} + \underbrace{(-i)\frac{1 \mp e^{-\beta\hbar\omega}}{2} J_1(\omega)}_{\text{imaginary part}}
\end{aligned}$$

Retarded and Finite-Temperature Green's Functions

- finite-temperature Green's function

$$\mathcal{G}^{\tau}(\tau) = -\langle \mathcal{T}_\tau \mathcal{A}(\tau)\mathcal{B}(0)\rangle = -\Theta(\tau)\langle \mathcal{A}(\tau)\mathcal{B}(0)\rangle \pm \Theta(-\tau)\langle \mathcal{B}(0)\mathcal{A}(\tau)\rangle \tag{73}$$

for $-\beta < \tau < \beta$, where

$$\mathcal{A}(\tau) = e^{\tau\mathcal{H}}\mathcal{A}e^{-\tau\mathcal{H}} \tag{74}$$

and τ is the imaginary time variable or the inverse temperature.

- correlation functions

$$\begin{aligned} \langle \mathcal{A}(\tau)\mathcal{B}(0)\rangle &= \sum_{nm} \frac{e^{-\beta E_m}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \langle m|\mathcal{A}|n\rangle e^{\tau(E_m - E_n)} \\ \langle \mathcal{B}(0)\mathcal{A}(\tau)\rangle &= \sum_{nm} \frac{e^{-\beta E_n}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \langle m|\mathcal{A}|n\rangle e^{\tau(E_m - E_n)} \end{aligned} \tag{75}$$

- periodicity of $\mathcal{G}^{\tau}(\tau)$: for $0 < \tau < \beta$,

$$\mathcal{G}^{\tau}(\tau) = \mp\mathcal{G}^{\tau}(\tau - \beta) \tag{76}$$

where the upper/lower signs correspond to bosonic/fermionic operators.
$\rightarrow$ due to the periodicity property, $\mathcal{G}^{\tau}$ can be expanded in a Fourier series.

TI-28: proof of Eq. (76)

Retarded and Finite-Temperature Green's Functions (cont.)

TI-28: proof of Eq. (76)

We pick $0 < \tau < \beta$ or equivalently $-\beta < \tau - \beta < 0$,

$$\begin{aligned}
\mathcal{G}^{\tau}(\tau-\beta) &= \pm \langle \mathcal{B}(0)\mathcal{A}(\tau-\beta)\rangle = \pm \sum_{nm} \frac{e^{-\beta E_n}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \langle m|\mathcal{A}|n\rangle\, e^{(\tau-\beta)(E_m-E_n)} \\
&= \pm \sum_{nm} \frac{e^{-\beta E_n - \beta(E_m-E_n)}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \langle m|\mathcal{A}|n\rangle\, e^{\tau(E_m-E_n)} \\
&= \pm \sum_{nm} \frac{e^{-\beta E_m}}{\mathcal{Z}} \langle n|\mathcal{B}|m\rangle \langle m|\mathcal{A}|n\rangle\, e^{\tau(E_m-E_n)} \\
&= \pm \langle \mathcal{A}(\tau)\mathcal{B}(0)\rangle = \mp \mathcal{G}^{\tau}(\tau)
\end{aligned}$$

Retarded and Finite-Temperature Green's Functions (cont.)

- Fourier transform

$$\mathcal{G}^\tau(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n \tau} \mathcal{G}^\tau(\tau)$$
$$\mathcal{G}^\tau(\tau) = \frac{1}{\beta}\sum_n e^{-i\omega_n\tau}\mathcal{G}^\tau(i\omega_n) \tag{77}$$

The periodicity put constraints on possible values of Matsubara frequencies

$$\omega_n = \begin{cases} \frac{(2n+1)\pi}{\beta}, & \text{fermions} \\ \frac{2n\pi}{\beta}, & \text{bosons} \end{cases} \tag{78}$$

- $\mathcal{G}^\tau(i\omega_n)$ in terms of $J_1(\omega)$

$$\mathcal{G}^\tau(i\omega_n) = \frac{1}{\hbar}\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{1 \pm e^{-\beta\hbar\omega'}}{i\omega_n/\hbar - \omega'} J_1(\omega') \tag{79}$$

TI-29: proof of Eq. (79)

Retarded and Finite-Temperature Green's Functions (cont.)

TI-29: proof of Eq. (79)

$$\begin{aligned}
\mathcal{G}^\tau(i\omega_n) &= \int_0^\beta d\tau\, e^{i\omega_n\tau}\mathcal{G}^\tau(\tau) = -\int_0^\beta d\tau\, e^{i\omega_n\tau}\,\langle\mathcal{A}(\tau)\mathcal{B}(0)\rangle \\
&= -\int_0^\beta d\tau\, e^{i\omega_n\tau}\sum_{nm}\frac{e^{-\beta E_m}}{\mathcal{Z}}\,\langle n|\mathcal{B}|m\rangle\,\langle m|\mathcal{A}|n\rangle\, e^{\tau(E_m-E_n)} \\
&= -\sum_{nm}\frac{e^{-\beta E_m}}{\mathcal{Z}}\,\langle n|\mathcal{B}|m\rangle\,\langle m|\mathcal{A}|n\rangle\int_0^\beta d\tau\, e^{(i\omega_n+E_m-E_n)\tau} \\
&= -\sum_{nm}\frac{e^{-\beta E_m}}{\mathcal{Z}}\,\langle n|\mathcal{B}|m\rangle\,\langle m|\mathcal{A}|n\rangle\,\frac{\mp e^{(E_m-E_n)\beta}-1}{i\omega_n+E_m-E_n}
\end{aligned}$$

since

$$e^{i\omega_n\beta} = \begin{cases} e^{i(2n+1)\pi} = -1, & \text{fermion} \\ e^{i(2n)\pi} = 1, & \text{boson} \end{cases}$$

And

$$\begin{aligned}
\mathcal{G}^\tau(i\omega_n) &= \int_{-\infty}^{\infty} d(\hbar\omega')\underbrace{\sum_{nm}\frac{e^{-\beta E_m}}{\mathcal{Z}}\,\langle n|\mathcal{B}|m\rangle\,\langle m|\mathcal{A}|n\rangle\,\delta(\hbar\omega'+E_m-E_n)}_{=J_1(\omega)/2\pi\hbar}\frac{1\pm e^{-\beta\hbar\omega'}}{i\omega_n-\hbar\omega'} \\
&= \frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\frac{1\pm e^{-\beta\hbar\omega'}}{i\omega_n/\hbar-\omega'}J_1(\omega')
\end{aligned}$$

Retarded and Finite-Temperature Green's Functions (cont.)

- analytical continuation

$$\mathcal{G}^\tau(i\omega_n) = \frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{1\pm e^{-\beta\hbar\omega'}}{i\omega_n/\hbar-\omega'}J_1(\omega')$$
$$\mathcal{G}^R(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{1\pm e^{-\beta\hbar\omega'}}{\omega-\omega'+i\eta}J_1(\omega') \tag{80}$$

$$\rightarrow \qquad \hbar\mathcal{G}^\tau(i\omega_n/\hbar\rightarrow\omega+i\eta)=\mathcal{G}^R(\omega) \tag{81}$$

» $\mathcal{G}^\tau(i\omega_n)$ is defined only at a discrete set of points $(i\omega_n)$ on the imaginary axis of frequency

» $\mathcal{G}^R(\omega)$ is defined for all values of ω in the real axis

» it is easier to calculate the finite-temperature Green's function compared to the retarded Green's function because the Wick's theorem can be applied to the finite-temperature Green's function

Electrical Conductivity

- our strategy: electrical conductivity $\sigma_{ss'}(\mathbf{q}, \omega)$
  $\leftarrow$ retarded Green's function $\mathcal{D}^R_{ss'}(\mathbf{q}, \omega)$ from Eq. (62)
  $\leftarrow$ (analytical continuation) finite-temperature Green's function $\mathcal{D}_{ss'}(\mathbf{q}, \tau)$
- remark on diamagnetic term
  - current contains a diamagnetic part (which is very important in obtaining the electromagnetic response of superconductors as well as the correct response of metals)

$$\mathbf{J}_e(\mathbf{r}, t) = \frac{in_0 e^2}{m\omega}\mathbf{E}(\mathbf{r}, t) \tag{82}$$

  - the first-order expansion in **A** neglects the diamagnetic part
  - it is diagonal in space indices and does not contribute to the Hall conductivity or other topological invariants of insulators $\rightarrow$ it is not taken into account in the following calculations
- spatial translational symmetry $\rightarrow$ Fourier transform over the position coordinates

$$\mathcal{D}^R_{ss'}(\mathbf{q}, t - t') = -i\Theta(t)\,\langle[\mathbf{j}_s(\mathbf{q}, t), \mathbf{j}_{s'}(-\mathbf{q}, t')]\rangle_0 \tag{83}$$

see Eq. (60).

Electrical Conductivity (cont.)

- finite-temperature Green's function

$$\mathcal{D}_{ss'}(\mathbf{q}, \tau - \tau') = -\langle \mathcal{T}_\tau \mathbf{j}_s(\mathbf{q}, \tau) \mathbf{j}_{s'}(-\mathbf{q}, \tau') \rangle_0 \tag{84}$$

  for $\tau - \tau' \geq 0$.
  - currents being bilinear in fermionic operators $\rightarrow$ bosonic operator
  - $\mathcal{D}_{ss'}(\mathbf{q}, \tau) = \mathcal{D}_{ss'}(\mathbf{q}, \tau + \beta)$
  - Matsubara frequency $\nu_n = 2n\pi/\beta$ for integer n
  - $\mathcal{D}_{ss'}$ depends only on $\tau - \tau'$, so we put $\tau' = 0$.
- imaginary-time-dependent current operator in the small q limit: from Eq. (46)

$$j_s(\mathbf{q}, \tau) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\alpha\beta} \frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial \hbar k_s} c^\dagger_{\mathbf{k}-\mathbf{q}/2\alpha}(\tau) c_{\mathbf{k}+\mathbf{q}/2\beta}(\tau) \tag{85}$$

  with $c(\tau) = e^{\tau\mathcal{H}} c e^{-\tau\mathcal{H}}$.

Electrical Conductivity (cont.)

- Wick's theorem ← non-interacting Hamiltonian (quadratic in c)

$$
\begin{aligned}
&\mathcal{D}_{ss'}(\mathbf{q},\tau) \\
&= -\frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\sum_{\alpha\beta\alpha'\beta'}\frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial \hbar k_s}\frac{\partial h_{\mathbf{k}'}^{\alpha'\beta'}}{\partial \hbar k'_{s'}}\left\langle \mathcal{T}_\tau c^\dagger_{\mathbf{k}-\mathbf{q}/2\alpha}(\tau)c_{\mathbf{k}+\mathbf{q}/2\beta}(\tau)c^\dagger_{\mathbf{k}'+\mathbf{q}/2\alpha'}c_{\mathbf{k}'-\mathbf{q}/2\beta'}\right\rangle_0 \\
&= -\frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\sum_{\alpha\beta\alpha'\beta'}\frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial \hbar k_s}\frac{\partial h_{\mathbf{k}'}^{\alpha'\beta'}}{\partial \hbar k'_{s'}}\left\langle \mathcal{T}_\tau c^\dagger_{\mathbf{k}-\mathbf{q}/2\alpha}(\tau)c_{\mathbf{k}'-\mathbf{q}/2\beta'}\right\rangle_0\left\langle \mathcal{T}_\tau c_{\mathbf{k}+\mathbf{q}/2\beta}(\tau)c^\dagger_{\mathbf{k}'+\mathbf{q}/2\alpha'}\right\rangle_0
\end{aligned}
\tag{86}
$$

Here we keep only the connected parts.

- fermionic finite-temperature Green's function

$$
\mathcal{G}_{\alpha\beta}(\mathbf{k},\tau) = -\left\langle \mathcal{T}_\tau c_{\mathbf{k}\alpha'}(\tau)c^\dagger_{\mathbf{k}\alpha}\right\rangle_0 \quad\rightarrow\quad \mathcal{G}_{\alpha\beta}(\mathbf{k},i\omega_n) = \left[\frac{1}{i\omega_n - h_{\mathbf{k}}}\right]_{\alpha\beta} \tag{87}
$$

here $\mathcal{G}(\mathbf{k},i\omega_n)$ is a $M\times M$ matrix.

Electrical Conductivity (cont.)

- Fourier transform

$$\mathcal{D}_{ss'}(\mathbf{q}, i\nu_n) = \frac{1}{N}\frac{1}{\beta}\sum_{\mathbf{k}}\sum_{m} \mathrm{Tr}\left[\frac{\partial h_{\mathbf{k}}}{\partial \hbar k_s}\mathcal{G}(\mathbf{k}+\mathbf{q}/2, i\omega_m)\frac{\partial h_{\mathbf{k}}}{\partial \hbar k_{s'}}\mathcal{G}(\mathbf{k}-\mathbf{q}/2, i\omega_m - i\nu_n)\right] \tag{88}$$

where the trace is done over the orbital indices.

TI-30: proof of Eq. (88)

- summation over Matsubara frequencies ω_m
- analytical continuation: $i\nu_n/\hbar \to \omega + i\eta$

Electrical Conductivity (cont.)

TI-30: proof of Eq. (88)

$$
\begin{aligned}
&\mathcal{D}_{ss'}(\mathbf{q}, i\nu_n) \\
&= \int_0^\beta d\tau\, e^{i\nu_n\tau}\mathcal{D}_{ss'}(\mathbf{q},\tau) \\
&= -\frac{1}{N}\int_0^\beta d\tau\, e^{i\nu_n\tau}\sum_{\mathbf{k}\mathbf{k}'}\sum_{\alpha\beta\alpha'\beta'}\frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial\hbar k_s}\frac{\partial h_{\mathbf{k}'}^{\alpha'\beta'}}{\partial\hbar k'_{s'}}\left\langle\mathcal{T}_\tau c^\dagger_{\mathbf{k}-\mathbf{q}/2\alpha}(\tau)c_{\mathbf{k}'-\mathbf{q}/2\beta'}\right\rangle_0\left\langle\mathcal{T}_\tau c_{\mathbf{k}+\mathbf{q}/2\beta}(\tau)c^\dagger_{\mathbf{k}'+\mathbf{q}/2\alpha'}\right\rangle_0 \\
&= -\frac{1}{N}\sum_{\mathbf{k}}\sum_{\alpha\beta\alpha'\beta'}\frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial\hbar k_s}\frac{\partial h_{\mathbf{k}}^{\alpha'\beta'}}{\partial\hbar k_{s'}}\int_0^\beta d\tau\, e^{i\nu_n\tau}\mathcal{G}_{\beta'\alpha}(\mathbf{k}-\mathbf{q}/2,-\tau)(-\mathcal{G}_{\beta\alpha'}(\mathbf{k}+\mathbf{q}/2,\tau)) \\
&= \frac{1}{N}\sum_{\mathbf{k}}\sum_{\alpha\beta\alpha'\beta'}\frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial\hbar k_s}\frac{\partial h_{\mathbf{k}}^{\alpha'\beta'}}{\partial\hbar k_{s'}}\int_0^\beta d\tau\, e^{i\nu_n\tau} \\
&\quad\times\frac{1}{\beta}\sum_{m'}e^{i\omega_{m'}\tau}\mathcal{G}_{\beta'\alpha}(\mathbf{k}-\mathbf{q}/2,i\omega_{m'})\frac{1}{\beta}\sum_m e^{-i\omega_m\tau}\mathcal{G}_{\beta\alpha'}(\mathbf{k}+\mathbf{q}/2,i\omega_m) \\
&= \frac{1}{N}\frac{1}{\beta}\sum_{mm'}\sum_{\mathbf{k}}\sum_{\alpha\beta\alpha'\beta'}\frac{\partial h_{\mathbf{k}}^{\alpha\beta}}{\partial\hbar k_s}\mathcal{G}_{\beta\alpha'}(\mathbf{k}+\mathbf{q}/2,i\omega_m)\frac{\partial h_{\mathbf{k}}^{\alpha'\beta'}}{\partial\hbar k_{s'}}\mathcal{G}_{\beta'\alpha}(\mathbf{k}-\mathbf{q}/2,i\omega_{m'})\underbrace{\frac{1}{\beta}\int_0^\beta d\tau\, e^{i(\nu_n+\omega_{m'}-\omega_m)\tau}}_{=\delta_{\omega_{m'},\omega_m-\nu_n}} \\
&= \frac{1}{N}\frac{1}{\beta}\sum_{\mathbf{k}}\sum_m \mathrm{Tr}\left[\frac{\partial h_{\mathbf{k}}}{\partial\hbar k_s}\mathcal{G}(\mathbf{k}+\mathbf{q}/2,i\omega_m)\frac{\partial h_{\mathbf{k}}}{\partial\hbar k_{s'}}\mathcal{G}(\mathbf{k}-\mathbf{q}/2,i\omega_m-i\nu_n)\right]
\end{aligned}
$$

Outline

Diagonalization of Hamiltonian

- energy eigenstates and eigenvalues of $M \times M$ matrix $h_{\mathbf{k}}^{\alpha\beta}$

$$h_{\mathbf{k}}^{\alpha\beta} u_{\beta}^{\gamma}(\mathbf{k}) = \epsilon_{\gamma}(\mathbf{k}) u_{\alpha}^{\gamma}(\mathbf{k}) \tag{89}$$

  - » $\epsilon_{\gamma}(\mathbf{k})$: $\gamma^{\rm th}$ energy eigenvalue ($\gamma = 1, \cdots, M$)
  - » $u_{\alpha}^{\gamma}(\mathbf{k})$: α component of $\gamma^{\rm th}$ orthonormal eigenstate

- unitary matrix $U(\mathbf{k})$

$$U_{\alpha\beta}(\mathbf{k}) = u_{\alpha}^{\beta}(\mathbf{k}) \quad \rightarrow \quad [U^{\dagger} U]_{\alpha\beta} = \sum_{\gamma} U_{\gamma\alpha}^{*} U_{\gamma\beta} = \sum_{\gamma} u_{\gamma}^{\alpha *} u_{\gamma}^{\beta} = \delta_{\alpha\beta} \tag{90}$$

$\leftarrow$ $\beta^{\rm th}$ column of $U(\mathbf{k})$ is the column vector by $u^{\beta}(\mathbf{k})$.

- diagonalization of $h_{\mathbf{k}}$

$$U^{\dagger}(\mathbf{k}) h_{\mathbf{k}} U(\mathbf{k}) = \mathrm{diag}(\epsilon_1(\mathbf{k}), \cdots, \epsilon_M(\mathbf{k})) \equiv \epsilon(\mathbf{k}) \tag{91}$$

- unitary transformation and diagonalization of $\mathcal{H}(\mathbf{k})$

$$\mathcal{H}(\mathbf{k}) = \sum_{\alpha} d_{\mathbf{k}\alpha}^{\dagger} \epsilon_{\alpha}(\mathbf{k}) d_{\mathbf{k}\alpha} \quad \text{with} \quad d_{\mathbf{k}\alpha} = \sum_{\beta} U_{\alpha\beta}^{\dagger}(\mathbf{k}) c_{\mathbf{k}\beta} \tag{92}$$

TI-31: proof of Eq. (92)

Diagonalization of Hamiltonian (cont.)

TI-31: proof of Eq. (92)

Using

$$U^\dagger(\mathbf{k}) h_\mathbf{k} U(\mathbf{k}) = \epsilon(\mathbf{k}) \quad \rightarrow \quad h_\mathbf{k} = U(\mathbf{k})\epsilon(\mathbf{k})U^\dagger(\mathbf{k})$$

one obtains

$$\begin{aligned}
\mathcal{H} &= \sum_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha} h^{\alpha\beta}_\mathbf{k} c_{\mathbf{k}\beta} \\
&= \sum_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha} \sum_\gamma U_{\alpha\gamma}(\mathbf{k})\epsilon_\gamma(\mathbf{k})U^\dagger_{\gamma\beta}(\mathbf{k})c_{\mathbf{k}\beta} \\
&= \sum_\gamma \left(\sum_\alpha U_{\alpha\gamma}(\mathbf{k}) c^\dagger_{\mathbf{k}\alpha} \right) \epsilon_\gamma(\mathbf{k}) \left(\sum_\beta U^\dagger_{\gamma\beta}(\mathbf{k}) c_{\mathbf{k}\beta} \right) \\
&= \sum_\gamma \underbrace{\left(\sum_\alpha U^\dagger_{\gamma\alpha}(\mathbf{k}) c_{\mathbf{k}\alpha} \right)^\dagger}_{= d^\dagger_{\mathbf{k}\gamma}} \epsilon_\gamma(\mathbf{k}) \underbrace{\left(\sum_\beta U^\dagger_{\gamma\beta}(\mathbf{k}) c_{\mathbf{k}\beta} \right)}_{= d_{\mathbf{k}\gamma}}
\end{aligned}$$

Adiabatic Transformation and Topological Properties

- linear-response electrical conductivity depends on the band energies, $\epsilon_\alpha(\mathbf{k})$ as well as the eigenstates
  $\leftarrow$ poles at $\epsilon_\alpha(\mathbf{k})$ of Green's functions $\rightarrow$ residue at each pole
- small adiabatic change of Hamiltonian (no gap is closed, no level crossing)
  $\rightarrow$ change in band energies
  $\rightarrow$ change in Hall conductance ?
- topological properties, if any, should not depend on the energies of the filled bands
  - if the (small) adiabatic change in the Hamiltonian affects the Hall conductance, it would not be topological invariant.
  - the immunity of the Hall conductance to the adiabatic change
    $\rightarrow$ a hint that it is a true topological quantity
  - the Hall conductance can depend on eigenstates: note that the Berry phase is determined by the adiabatic evolution of eigenstates.
- flat-band limit
  - the energy of all the occupied states set to be a same value, say $\epsilon_G < 0$ (note that currently the chemical potential is set to be zero)
  - the energy of all the unoccupied states set to be a same value, say $\epsilon_E > 0$

  $\rightarrow$ makes it easier to calculate the conductivity while the topological nature is still captured.

Flat-Band Limit

- ordering of band energies: p filled bands and $M - p$ empty bands

$$\epsilon_1(\mathbf{k}) \le \epsilon_2(\mathbf{k}) \le \cdots \le \epsilon_p(\mathbf{k}) < 0(= \mu) < \epsilon_{p+1}(\mathbf{k}) \le \cdots \le \epsilon_M(\mathbf{k}) \tag{93}$$

  insulator $\rightarrow$ we assume that all the empty bands are separated by a full gap at all $\mathbf{k}$ from the filled (negative-energy) bands

- adiabatic transformation: for an adiabatic parameter $t \in [0, 1]$

$$E_\alpha(\mathbf{k}, t) = \begin{cases} \epsilon_\alpha(\mathbf{k})(1 - t) + \epsilon_G t, & 1 \le \alpha \le p \\ \epsilon_\alpha(\mathbf{k})(1 - t) + \epsilon_E t, & p + 1 \le \alpha \le M \end{cases} \tag{94}$$

  » at $t = 0$, $E_\alpha(\mathbf{k}, 0) = \epsilon_\alpha(\mathbf{k})$
  » at $t = 1$, $E_\alpha(\mathbf{k}, t) = \epsilon_G$ for $\alpha \le p$ and ϵ_E for $\alpha \ge p + 1$
  » throughout the adiabatic evolution, the structure of the band energies remains same: (1) the Hamiltonian remains gapped and (2) no band crossing at the Fermi level
  » BUT this transformation keeps the eigenstates from changing

$$h_\mathbf{k}(t) = U(\mathbf{k})\mathrm{diag}(E_1(\mathbf{k}, t), \cdots, E_M(\mathbf{k}, t))U^\dagger(\mathbf{k}) \tag{95}$$

  » we are interested in only the final transformation at $t = 1$

Flat-Band Limit (cont.)

- Hamiltonian after the adiabatic transformation for **k**

$$h_{\mathbf{k}}(t=1) = \epsilon_G \sum_{\alpha=1}^{p} |\alpha\mathbf{k}\rangle \langle\alpha\mathbf{k}| + \epsilon_E \sum_{\alpha=p+1}^{M} |\alpha\mathbf{k}\rangle \langle\alpha\mathbf{k}|, \quad \text{where} \quad |\alpha\mathbf{k}\rangle = d^{\dagger}_{\mathbf{k}\alpha} |0\rangle \tag{96}$$

- projection operator to γ^{th} eigenstate

$$\mathcal{P}^{\gamma}(\mathbf{k}) \equiv |\gamma\mathbf{k}\rangle \langle\gamma\mathbf{k}| \quad \rightarrow \quad \mathcal{P}^{\gamma}_{\alpha\beta}(\mathbf{k}) = \langle\alpha|\gamma\mathbf{k}\rangle \langle\gamma\mathbf{k}|\beta\rangle = u^{\gamma}_{\alpha}(\mathbf{k}) u^{\gamma *}_{\beta}(\mathbf{k}) \tag{97}$$

satisfying

$$\mathcal{P}^{\gamma}(\mathbf{k}) \sum_{\gamma'} a_{\gamma'} |\gamma'\mathbf{k}\rangle = \sum_{\gamma'} a_{\gamma'} |\gamma\mathbf{k}\rangle \langle\gamma\mathbf{k}|\gamma'\mathbf{k}\rangle = a_{\gamma} |\gamma\mathbf{k}\rangle \tag{98}$$

- projection operators to filled and empty bands

$$\mathcal{P}^{G}(\mathbf{k}) \equiv \sum_{\alpha=1}^{p} |\alpha\mathbf{k}\rangle \langle\alpha\mathbf{k}| \quad \text{and} \quad \mathcal{P}^{E}(\mathbf{k}) \equiv \sum_{\alpha=p+1}^{M} |\alpha\mathbf{k}\rangle \langle\alpha\mathbf{k}| \tag{99}$$

satisfying the following identities:

$$h_{\mathbf{k}}(1) = \epsilon_G \mathcal{P}^{G}(\mathbf{k}) + \epsilon_E \mathcal{P}^{E}(\mathbf{k}), \quad \mathcal{P}^{G} + \mathcal{P}^{E} = 1, \quad [\mathcal{P}^{G/E}]^2 = \mathcal{P}^{G/E}, \quad \mathcal{P}^{G}\mathcal{P}^{E} = 0 \tag{100}$$

Flat-Band Limit (cont.)

- fermionic finite-temperature Green's function

$$\mathcal{G}(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n - h_{\mathbf{k}}(1)} = \frac{\mathcal{P}^G(\mathbf{k})}{i\omega_n - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_n - \epsilon_E} \tag{101}$$

TI-32: proof of Eq. (101)

- current-current correlation function (finite-temperature Green's function for current) from Eq. (88) in the $\mathbf{q} \to 0$ limit

$$\begin{aligned}\mathcal{D}_{ss'}(\mathbf{q} \to 0, i\nu_n) = \frac{(\epsilon_G - \epsilon_E)^2}{N\beta} \sum_{\mathbf{k}} \sum_m \mathrm{Tr}\Bigg[&\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s} \left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - \epsilon_E} \right) \\ \times &\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_{s'}} \left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_E} \right) \Bigg]\end{aligned} \tag{102}$$

TI-33: proof of Eq. (102)

Flat-Band Limit (cont.)

TI-32: proof of Eq. (101)

Since (omitting the argument **k** for $\mathcal{P}^{G/E}$ for simplicity)

$$\begin{aligned}\left(\frac{\mathcal{P}^G}{i\omega_n - \epsilon_G} + \frac{\mathcal{P}^E}{i\omega_n - \epsilon_E}\right)(i\omega_n - h_{\mathbf{k}}) &= \left(\frac{\mathcal{P}^G}{i\omega_n - \epsilon_G} + \frac{\mathcal{P}^E}{i\omega_n - \epsilon_E}\right)\left(i\omega_n - \epsilon_G\mathcal{P}^G - \epsilon_E\mathcal{P}^E\right) \\ &= \frac{\mathcal{P}^G i\omega_n - \mathcal{P}^{G2}\epsilon_G}{i\omega_n - \epsilon_G} + \frac{\mathcal{P}^E i\omega_n - \mathcal{P}^{E2}\epsilon_E}{i\omega_n - \epsilon_E} \quad (\because \mathcal{P}^E\mathcal{P}^G = 0) \\ &= \mathcal{P}^G + \mathcal{P}^E \quad (\because \mathcal{P}^{G2} = \mathcal{P}^G,\ \mathcal{P}^{E2} = \mathcal{P}^E) \\ &= 1,\end{aligned}$$

one finds that

$$\mathcal{G}(\mathbf{k}, i\omega_n) = (i\omega_n - h_{\mathbf{k}})^{-1} = \frac{\mathcal{P}^G(\mathbf{k})}{i\omega_n - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_n - \epsilon_E}$$

Flat-Band Limit (cont.)

TI-33: proof of Eq. (102)

Since, at $t = 1$,

$$\frac{\partial h_{\mathbf{k}}(1)}{\partial \hbar k_s} = \frac{\partial}{\partial \hbar k_s}\left(\epsilon_G \mathcal{P}^G(\mathbf{k}) + \epsilon_E \mathcal{P}^E(\mathbf{k})\right) = \epsilon_G \frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s} + \epsilon_E \frac{\partial}{\partial \hbar k_s}(1 - \mathcal{P}^G(\mathbf{k})) = (\epsilon_G - \epsilon_E)\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s}$$

and using the fermionic finite-temperature Green's function given by Eq. (101), the current-current correlation function (in its Fourier transform) is simplified into

$$\begin{aligned}
\mathcal{D}_{ss'}(\mathbf{q} \to 0, i\nu_n) &= \frac{1}{N\beta}\sum_{\mathbf{k}}\sum_m \mathrm{Tr}\left[\frac{\partial h_{\mathbf{k}}}{\partial \hbar k_s}\mathcal{G}(\mathbf{k}, i\omega_m)\frac{\partial h_{\mathbf{k}}}{\partial \hbar k_{s'}}\mathcal{G}(\mathbf{k}, i\omega_m - i\nu_n)\right] \\
&= \frac{1}{N\beta}\sum_{\mathbf{k}}\sum_m \mathrm{Tr}\left[(\epsilon_G - \epsilon_E)\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s}\left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - \epsilon_E}\right)\right. \\
&\qquad \left. \times (\epsilon_G - \epsilon_E)\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_{s'}}\left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_E}\right)\right] \\
&= \frac{(\epsilon_G - \epsilon_E)^2}{N\beta}\sum_{\mathbf{k}}\sum_m \mathrm{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s}\left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - \epsilon_E}\right)\right. \\
&\qquad \left. \times \frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_{s'}}\left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_E}\right)\right]
\end{aligned}$$

Flat-Band Limit (cont.)

- projector algebra

$$(\partial_s\mathcal{P}^G)\mathcal{P}^G(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G = (\partial_s\mathcal{P}^G)\mathcal{P}^E(\partial_{s'}\mathcal{P}^G)\mathcal{P}^E = 0 \tag{103a}$$
$$(\partial_s\mathcal{P}^G)\mathcal{P}^G(\partial_{s'}\mathcal{P}^G)\mathcal{P}^E = -(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^E)\mathcal{P}^E \tag{103b}$$
$$(\partial_s\mathcal{P}^G)\mathcal{P}^E(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G = -(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^E)\mathcal{P}^G \tag{103c}$$

TI-34: proof of Eq. (103)

- summation over Matsubara frequency ω_m

$$\mathcal{D}_{ss'}(\mathbf{q}\to 0, i\nu_n) = \frac{(\epsilon_G-\epsilon_E)^2}{N}(n_F(\epsilon_G)-n_F(\epsilon_E)) \times \sum_{\mathbf{k}}\left(\frac{\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_s}\frac{\partial\mathcal{P}^E(\mathbf{k})}{\partial\hbar k_{s'}}\mathcal{P}^G(\mathbf{k})\right]}{i\nu_n+\epsilon_G-\epsilon_E} - \frac{\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_s}\frac{\partial\mathcal{P}^E(\mathbf{k})}{\partial\hbar k_{s'}}\mathcal{P}^E(\mathbf{k})\right]}{i\nu_n+\epsilon_E-\epsilon_G}\right) \tag{104}$$

TI-35: proof of Eq. (104)

Flat-Band Limit (cont.)

TI-34: proof of Eq. (103)

For simplicity, we omit the argument **k** for $\mathcal{P}^{G/E}$.

First, we derive some nice identities:

$$
\begin{aligned}
1 = \mathcal{P}^G + \mathcal{P}^E &\to \quad 0 = \partial_s(\mathcal{P}^G + \mathcal{P}^E) \quad \to \quad \partial_s\mathcal{P}^G = -\partial_s\mathcal{P}^E && \text{(a)}\\
0 = \mathcal{P}^E\mathcal{P}^G &\to \quad 0 = \partial_s(\mathcal{P}^E\mathcal{P}^G) \quad \to \quad (\partial_s\mathcal{P}^E)\mathcal{P}^G = -\mathcal{P}^E\partial_s\mathcal{P}^G && \text{(b)}\\
\mathcal{P}^{G/E} = [\mathcal{P}^{G/E}]^2 &\to \quad \partial_s\mathcal{P}^{G/E} = (\partial_s\mathcal{P}^{G/E})\mathcal{P}^{G/E} + \mathcal{P}^{G/E}\partial_s\mathcal{P}^{G/E} \\
&\to \quad \mathcal{P}^{G/E}\partial_s\mathcal{P}^{G/E} = \partial_s\mathcal{P}^{G/E} - (\partial_s\mathcal{P}^{G/E})\mathcal{P}^{G/E} && \text{(c)}
\end{aligned}
$$

- $(\partial_s\mathcal{P}^G)\mathcal{P}^G(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G$

$$
\begin{aligned}
(\partial_s\mathcal{P}^G)\mathcal{P}^G(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G &= (\partial_s\mathcal{P}^G)\left(\partial_{s'}\mathcal{P}^G - (\partial_{s'}\mathcal{P}^G)\mathcal{P}^G\right)\mathcal{P}^G \quad (\because \text{Eq. (c)})\\
&= (\partial_s\mathcal{P}^G)\left((\partial_{s'}\mathcal{P}^G)\mathcal{P}^G - (\partial_{s'}\mathcal{P}^G)\mathcal{P}^G\right) \quad (\because [\mathcal{P}^G]^2 = \mathcal{P}^G)\\
&= 0
\end{aligned}
$$

- $(\partial_s\mathcal{P}^G)\mathcal{P}^E(\partial_{s'}\mathcal{P}^G)\mathcal{P}^E$

$$
\begin{aligned}
(\partial_s\mathcal{P}^G)\mathcal{P}^E(\partial_{s'}\mathcal{P}^G)\mathcal{P}^E &= (\partial_s\mathcal{P}^G)\left(-(\partial_{s'}\mathcal{P}^E)\mathcal{P}^G\right)\mathcal{P}^E \quad (\because \text{Eq. (b)})\\
&= 0 \quad (\because \mathcal{P}^G\mathcal{P}^E = 0)
\end{aligned}
$$

Flat-Band Limit (cont.)

- $(\partial_s \mathcal{P}^G)\mathcal{P}^G(\partial_{s'}\mathcal{P}^G)\mathcal{P}^E$

$$\begin{aligned}
(\partial_s \mathcal{P}^G)\mathcal{P}^G(\partial_{s'}\mathcal{P}^G)\mathcal{P}^E &= (\partial_s \mathcal{P}^G)\mathcal{P}^G(-\partial_{s'}\mathcal{P}^E)\mathcal{P}^E \quad (\because \text{Eq. (a)}) \\
&= (\partial_s \mathcal{P}^G)(\partial_{s'}\mathcal{P}^G)\mathcal{P}^E\mathcal{P}^E \quad (\because \text{Eq. (b)}) \\
&= -(\partial_s \mathcal{P}^G)(\partial_{s'}\mathcal{P}^E)\mathcal{P}^E \quad (\because \text{Eq. (a) and } [\mathcal{P}^E]^2 = \mathcal{P}^E)
\end{aligned}$$

- $(\partial_s \mathcal{P}^G)\mathcal{P}^E(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G$

$$\begin{aligned}
(\partial_s \mathcal{P}^G)\mathcal{P}^E(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G &= (\partial_s \mathcal{P}^G)(-(\partial_{s'}\mathcal{P}^E)\mathcal{P}^G)\mathcal{P}^G \quad (\because \text{Eq. (b)}) \\
&= -(\partial_s \mathcal{P}^G)(\partial_{s'}\mathcal{P}^E)\mathcal{P}^G \quad (\because [\mathcal{P}^G]^2 = \mathcal{P}^G)
\end{aligned}$$

Flat-Band Limit (cont.)

TI-35: proof of Eq. (104)

Noticing that the fermionic Matsubara frequencies $i\omega_m$ are the poles of the Fermi-Dirac distribution function

$$n_F(z) = \frac{1}{e^{\beta z} + 1}$$

since $e^{\beta(i\omega_m)} = e^{i(2m+1)\pi} = -1$ and near the poles

$$\frac{1}{e^{\beta z}+1} \approx \frac{1}{\left.\frac{d e^{\beta z}}{dz}\right|_{z=i\omega_n}(z - i\omega_n)} = -\frac{1}{\beta}\frac{1}{z - i\omega_n}$$

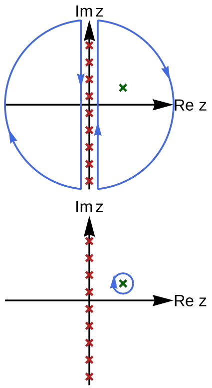
gives rise to a residue $-1/\beta$, a contour integral around one of the pole ($i\omega_m$) for an analytical function $g(z)$ is then

$$\oint \frac{dz}{2\pi i}(-\beta n_F(z))g(z) = g(i\omega_m).$$

Consider a counterclockwise contour integral along the contour C_1 surrounding the imaginary axis (see two straight lines in the upper figure) whose upper and lower segments should be vanishing due to infinitesimally small length of the corresponding integral interval. Since all the poles of $n_F(z)$ are enclosed by this contour,

$$\oint_{C_1} \frac{dz}{2\pi i}(-\beta n_F(z))g(z) = \sum_m g(i\omega_m).$$

By adding the circular contour integrals (see the upper figure) whose contribution should be zero, now we have two clockwise closed contour integrals which can be deformed to the contour C_2 going around the poles of $g(z)$ (see the lower figure).



Flat-Band Limit (cont.)

Therefore, the summation over the Matsubara frequencies can be accomplished by summing the residue of $(-\beta n_F(z))g(z)$ over the poles of $g(z)$ (say z_m):

$$\sum_m g(i\omega_m) = \oint_{C_1} \frac{dz}{2\pi i}(-\beta n_F(z))g(z) = \oint_{C_2} \frac{dz}{2\pi i}(-\beta n_F(z))g(z) = -\sum_m (-\beta n_F(z_m))\mathrm{Res}[g(z_m)]$$

where the minus sign comes from the fact that the contour C_2 is clockwise.

In our calculations, we need $g(z) = 1/(z - z_1)(z - z_2)$ where z_1 and $z_1 \neq z_2$ are complex constants. Then,

$$\begin{aligned}\frac{1}{\beta}\sum_m g(i\omega_m) &= \frac{1}{\beta}\sum_m \frac{1}{(i\omega_m - z_1)(i\omega_m - z_2)} = \frac{1}{z_2 - z_1}\frac{1}{\beta}\sum_m \left(\frac{1}{i\omega_m - z_1} - \frac{1}{i\omega_m - z_2}\right) \\ &= \frac{n_F(z_1) - n_F(z_2)}{z_2 - z_1} \qquad \text{(a)}\end{aligned}$$

since the residue of $1/(z - z_{1/2})$ at $z = z_{1/2}$ is one. Using Eq. (a) and the previous results in projector algebra, one gets

$$\begin{aligned}&\mathcal{D}_{ss'}(\mathbf{q} \to 0, i\nu_n) \\ &= \frac{(\epsilon_G - \epsilon_E)^2}{N\beta}\sum_{\mathbf{k}}\sum_m \mathrm{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s}\left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - \epsilon_E}\right)\right. \\ &\qquad \left. \times \frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_{s'}}\left(\frac{\mathcal{P}^G(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_G} + \frac{\mathcal{P}^E(\mathbf{k})}{i\omega_m - i\nu_n - \epsilon_E}\right)\right] \\ &= \frac{(\epsilon_G - \epsilon_E)^2}{N\beta}\sum_{\mathbf{k}}\sum_m \mathrm{Tr}\left[\frac{\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s}\mathcal{P}^E(\mathbf{k})\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_{s'}}\mathcal{P}^G(\mathbf{k})}{(i\omega_m - \epsilon_E)(i\omega_m - i\nu_n - \epsilon_G)} + \frac{\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s}\mathcal{P}^G(\mathbf{k})\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_{s'}}\mathcal{P}^E(\mathbf{k})}{(i\omega_m - \epsilon_G)(i\omega_m - i\nu_n - \epsilon_E)}\right]\end{aligned}$$

Flat-Band Limit (cont.)

$$= \frac{(\epsilon_G - \epsilon_E)^2}{N} \sum_{\mathbf{k}} \Bigg(- \operatorname{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s} \frac{\partial \mathcal{P}^E(\mathbf{k})}{\partial \hbar k_{s'}} \mathcal{P}^G(\mathbf{k}) \right] \frac{n_F(\epsilon_E) - n_F(i\nu_n + \epsilon_G)}{i\nu_n + \epsilon_G - \epsilon_E}$$
$$- \operatorname{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s} \frac{\partial \mathcal{P}^E(\mathbf{k})}{\partial \hbar k_{s'}} \mathcal{P}^E(\mathbf{k}) \right] \frac{n_F(\epsilon_G) - n_F(i\nu_n + \epsilon_E)}{i\nu_n + \epsilon_E - \epsilon_G} \Bigg)$$
$$= \frac{(\epsilon_G - \epsilon_E)^2}{N} (n_F(\epsilon_G) - n_F(\epsilon_E)) \sum_{\mathbf{k}} \left(\frac{\operatorname{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s} \frac{\partial \mathcal{P}^E(\mathbf{k})}{\partial \hbar k_{s'}} \mathcal{P}^G(\mathbf{k}) \right]}{i\nu_n + \epsilon_G - \epsilon_E} - \frac{\operatorname{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s} \frac{\partial \mathcal{P}^E(\mathbf{k})}{\partial \hbar k_{s'}} \mathcal{P}^E(\mathbf{k}) \right]}{i\nu_n + \epsilon_E - \epsilon_G} \right)$$

where in the last line we have used the fact that

$$n_F(i\nu_n + \epsilon) = \frac{1}{e^{\beta(i\nu_n)} e^{\beta\epsilon} + 1} = \frac{1}{e^{\beta\epsilon} + 1} = n_F(\epsilon)$$

since ν_n are the bosonic Matsubara frequencies satisfying $e^{\beta(i\nu_n)} = 1$.

Flat-Band Limit (cont.)

- analytical continuation, $i\nu_n \to \omega + i\eta$

$$\mathcal{D}^R_{ss'}(\mathbf{q} \to 0, \omega) = \hbar \mathcal{D}_{ss'}(\mathbf{q} \to 0, i\nu_n/\hbar \to \omega + i\eta) \tag{105}$$

- Hall conductivity or conductance
$\to$ only antisymmetric part with respect to directional indices s, s' is finite

$$\begin{aligned}\mathcal{D}^R_{ss'}(\mathbf{q} \to 0, \omega) = (n_F(\epsilon_G) - n_F(\epsilon_E)) \frac{2\omega(\epsilon_G - \epsilon_E)^2}{(\epsilon_G - \epsilon_E)^2/\hbar^2 - (\omega + i\eta)^2} \\ \times \frac{1}{N} \sum_{\mathbf{k}} \mathrm{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_s} \frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial \hbar k_{s'}} \mathcal{P}^G(\mathbf{k})\right]\end{aligned} \tag{106}$$

Note that we have now obtained the correlation function purely in terms of projection operators $\mathcal{P}^G$ into the ground-state manifold of occupied bands. Numerically, this is the way we compute the Hall conductance because projectors are manifestly gauge invariant, thereby bypassing the need for the gauge smoothing.

TI-36: proof of Eq. (106)

Flat-Band Limit (cont.)

TI-36: proof of Eq. (106)

$$\mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^E)\mathcal{P}^G\right] = \mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(-\partial_{s'}\mathcal{P}^G)\mathcal{P}^G\right] = -\,\mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G\right]$$

$$\mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^E)\mathcal{P}^E\right] = \mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(-\partial_{s'}\mathcal{P}^G)(1-\mathcal{P}^G)\right] = \mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^G)\mathcal{P}^G\right] - \mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^G)\right]$$

Note that the last term is symmetric in s and s' due to the property of the trace operation:

$$\mathrm{Tr}\left[(\partial_s\mathcal{P}^G)(\partial_{s'}\mathcal{P}^G)\right] = \mathrm{Tr}\left[(\partial_{s'}\mathcal{P}^G)(\partial_s\mathcal{P}^G)\right]$$

so it is neglected (it should vanish for $s \neq s'$). Therefore,

$$\begin{aligned}
&\mathcal{D}^R_{ss'}(\mathbf{q}\to 0,\omega)\\
&= \frac{\hbar}{\hbar}\frac{(\epsilon_G-\epsilon_E)^2}{N}(n_F(\epsilon_G)-n_F(\epsilon_E))\sum_{\mathbf{k}}\left(\frac{\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_s}\frac{\partial\mathcal{P}^E(\mathbf{k})}{\partial\hbar k_{s'}}\mathcal{P}^G(\mathbf{k})\right]}{\omega+i\eta+(\epsilon_G-\epsilon_E)/\hbar} - \frac{\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_s}\frac{\partial\mathcal{P}^E(\mathbf{k})}{\partial\hbar k_{s'}}\mathcal{P}^E(\mathbf{k})\right]}{\omega+i\eta+(\epsilon_E-\epsilon_G)/\hbar}\right)\\
&= \frac{(\epsilon_G-\epsilon_E)^2}{N}(n_F(\epsilon_G)-n_F(\epsilon_E))\left(-\frac{1}{\omega+i\eta+(\epsilon_G-\epsilon_E)/\hbar} - \frac{1}{\omega+i\eta+(\epsilon_E-\epsilon_G)/\hbar}\right)\\
&\quad\times\sum_{\mathbf{k}}\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_s}\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_{s'}}\mathcal{P}^G(\mathbf{k})\right]\\
&= (n_F(\epsilon_G)-n_F(\epsilon_E))\frac{2\omega(\epsilon_G-\epsilon_E)^2}{(\epsilon_G-\epsilon_E)^2/\hbar^2-(\omega+i\eta)^2}\frac{1}{N}\sum_{\mathbf{k}}\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_s}\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_{s'}}\mathcal{P}^G(\mathbf{k})\right]
\end{aligned}$$

Flat-Band Limit (cont.)

- Hall conductance: from Eqs. (62) and (71)

$$i\omega\sigma_{ss'}(\omega) = -\frac{e^2}{\hbar c}\mathcal{D}^R_{ss'}(\omega) \quad \to \quad \sigma_{ss'}(\omega) = \frac{e^2}{\hbar c}\frac{i}{\omega}\mathcal{D}^R_{ss'}(\omega) \tag{107}$$

here the constant c (due to cgs unit system) can be dropped in the MKS unit system.

- dc limit, $\omega \to 0$ and zero temperature, $T = 0$
  - » nonzero frequency corrections contain terms related to excitation into the empty bands
  - » finite-temperature corrections contain thermal fluctuations into the empty bands

$\Rightarrow$ only the zero-frequency and zero-temperature Hall conductivity has topological meaning

$$\sigma_{ss'} \equiv \sigma_{ss'}(\omega \to 0) = 2i\frac{e^2}{\hbar}\frac{1}{N}\sum_{\mathbf{k}} \mathrm{Tr}\left[\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial k_s}\frac{\partial \mathcal{P}^G(\mathbf{k})}{\partial k_{s'}}\mathcal{P}^G(\mathbf{k})\right] \tag{108}$$

TI-37: proof of Eq. (108)

Flat-Band Limit (cont.)

TI-37: proof of Eq. (108)

At zero temperature, $n_F(\epsilon_G < 0) = 1$ and $n_F(\epsilon_E > 0) = 0$. Therefore, at zero temperature and in the $\omega \to 0$ limit,

$$\begin{aligned}\sigma_{ss'}(\omega \to 0) &= \frac{e^2}{\hbar c}\frac{i}{\omega}\mathcal{D}^R_{ss'}(\omega)\\ &= \frac{e^2}{\hbar c}\frac{i}{\omega}(n_F(\epsilon_G) - n_F(\epsilon_E))\frac{2\omega(\epsilon_G-\epsilon_E)^2}{(\epsilon_G-\epsilon_E)^2/\hbar^2 - (\omega+i\eta)^2}\frac{1}{N}\sum_{\mathbf{k}}\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_s}\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial\hbar k_{s'}}\mathcal{P}^G(\mathbf{k})\right]\\ &= 2i\frac{e^2}{\hbar}\frac{1}{N}\sum_{\mathbf{k}}\mathrm{Tr}\left[\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial k_s}\frac{\partial\mathcal{P}^G(\mathbf{k})}{\partial k_{s'}}\mathcal{P}^G(\mathbf{k})\right]\end{aligned}$$

Flat-Band Limit (cont.)

- Hall conductance

$$\sigma_{xy} = \frac{e^2}{\hbar}\frac{1}{N}\sum_{\mathbf{k}}\sum_{\alpha=1}^{p}[F_\alpha(\mathbf{k})]_{xy} \tag{109}$$

in terms of the Berry curvature

$$[F_\alpha(\mathbf{k})]_{xy} = i\left(\langle\partial_x\alpha\mathbf{k}|\partial_y\alpha\mathbf{k}\rangle - \langle\partial_y\alpha\mathbf{k}|\partial_x\alpha\mathbf{k}\rangle\right) \tag{110}$$

TI-38: proof of Eq. (109)

- redefinition of Fourier transform: infinite lattice $\to$ Brillouin zone

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi}\underbrace{\int_{\mathrm{BZ}} dk_x dk_y \sum_{\alpha=1}^{p} F_{xy}(\alpha\mathbf{k})}_{=\text{ Berry phase}} \tag{111}$$

TI-39: proof of Eq. (111)

Flat-Band Limit (cont.)

TI-38: proof of Eq. (109)

$$\mathrm{Tr}\left[(\partial_s\mathcal{P}^G(\mathbf{k}))(\partial_{s'}\mathcal{P}^G(\mathbf{k}))\mathcal{P}^G(\mathbf{k})\right] = \sum_{\alpha=1}^{M}\langle\alpha\mathbf{k}|(\partial_s\mathcal{P}^G(\mathbf{k}))(\partial_{s'}\mathcal{P}^G(\mathbf{k}))\mathcal{P}^G(\mathbf{k})|\alpha\mathbf{k}\rangle$$

$$= \sum_{\alpha=1}^{p}\langle\alpha\mathbf{k}|(\partial_s\mathcal{P}^G(\mathbf{k}))(\partial_{s'}\mathcal{P}^G(\mathbf{k}))|\alpha\mathbf{k}\rangle$$

$$= \sum_{\alpha=1}^{p}\langle\alpha\mathbf{k}|\sum_{\beta=1}^{p}\Big(\partial_s\,|\beta\mathbf{k}\rangle\langle\beta\mathbf{k}| + |\beta\mathbf{k}\rangle\langle\partial_s\beta\mathbf{k}|\Big)\sum_{\gamma=1}^{p}\Big(\partial_{s'}\,|\gamma\mathbf{k}\rangle\langle\gamma\mathbf{k}| + |\gamma\mathbf{k}\rangle\langle\partial_{s'}\gamma\mathbf{k}|\Big)|\alpha\mathbf{k}\rangle$$

$$= \sum_{\alpha,\beta=1}^{p}\Big[\langle\alpha\mathbf{k}|\partial_s|\beta\mathbf{k}\rangle\langle\beta\mathbf{k}|\partial_{s'}|\alpha\mathbf{k}\rangle + \langle\alpha\mathbf{k}|\partial_s|\beta\mathbf{k}\rangle\langle\partial_{s'}\beta\mathbf{k}|\alpha\mathbf{k}\rangle\Big]$$

$$+ \sum_{\alpha=1}^{p}\langle\partial_s\alpha\mathbf{k}|\partial_{s'}|\alpha\mathbf{k}\rangle + \sum_{\alpha,\beta=1}^{p}\langle\partial_s\alpha\mathbf{k}|\beta\mathbf{k}\rangle\langle\partial_{s'}\beta\mathbf{k}|\alpha\mathbf{k}\rangle$$

$$= \sum_{\alpha=1}^{p}\langle\partial_s\alpha\mathbf{k}|\partial_{s'}|\alpha\mathbf{k}\rangle + \sum_{\alpha,\beta=1}^{p}\langle\alpha\mathbf{k}|\partial_s|\beta\mathbf{k}\rangle\langle\beta\mathbf{k}|\partial_{s'}|\alpha\mathbf{k}\rangle + \sum_{\alpha,\beta=1}^{p}(\partial_s\langle\alpha\mathbf{k}|\beta\mathbf{k}\rangle)\langle\partial_{s'}\beta\mathbf{k}|\alpha\mathbf{k}\rangle$$

$$= \sum_{\alpha=1}^{p}\langle\partial_s\alpha\mathbf{k}|\partial_{s'}|\alpha\mathbf{k}\rangle + \sum_{\alpha,\beta=1}^{p}\langle\alpha\mathbf{k}|\partial_s|\beta\mathbf{k}\rangle\langle\beta\mathbf{k}|\partial_{s'}|\alpha\mathbf{k}\rangle$$

where the second term is obviously symmetric in s and s' so that it should vanish.

Flat-Band Limit (cont.)

Since the Hall conductivity is antisymmetric, explicitly,

$$\begin{aligned}\sigma_{ss'} &= \frac{\sigma_{ss'} - \sigma_{s's}}{2} \\ &= \frac{e^2}{\hbar}\frac{1}{N}\sum_{\mathbf{k}}\sum_{\alpha=1}^{p}\left(i\left\langle\partial_s\alpha\mathbf{k}\middle|\partial_{s'}\middle|\alpha\mathbf{k}\right\rangle - i\left\langle\partial_{s'}\alpha\mathbf{k}\middle|\partial_s\middle|\alpha\mathbf{k}\right\rangle\right) \\ &= \frac{e^2}{\hbar}\frac{1}{N}\sum_{\mathbf{k}}\sum_{\alpha=1}^{p}[F_\alpha(\mathbf{k})]_{ss'}\end{aligned}$$

Flat-Band Limit (cont.)

TI-39: proof of Eq. (111)

For simplicity, here we assume an infinite one-dimensional lattice system. Then, the Fourier transform is defined as

$$c_{k_x} = \frac{1}{\sqrt{2\pi}} \sum_{n_x} e^{-ik_x n_x} c_{n_x} \quad \text{and} \quad c_{n_x} = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dk_x\, e^{ik_x n_x} c_{k_x}$$

for $-\pi < k_x \leq \pi$. Note that c_{k_x} is periodic in k_x by 2π:

$$c_{k_x+2\pi} = \sum_{n_x} e^{-i(k_x+2\pi)n_x} c_{n_x} = \sum_{n_x} e^{-ik_x n_x} e^{-2\pi i n_x} c_{n_x} = c_{k_x}$$

With this Fourier transform, the previous calculations can be properly modified. For example, the Hamiltonian is transformed into

$$\begin{aligned}
\mathcal{H} &= \sum_{ij} \sum_{\alpha\beta} c^\dagger_{i\alpha} h^{\alpha\beta}_{ij} c_{j\beta} = \sum_{ij} \sum_{\alpha\beta} \frac{1}{\sqrt{2\pi}} \int dk_x e^{-ik_x n_i} c^\dagger_{k_x\alpha} h^{\alpha\beta}_{ij} \frac{1}{\sqrt{2\pi}} \int dq_x e^{iq_x n_j} c_{q_x\beta} \\
&= \int dk_x \int dq_x \sum_{\alpha\beta} c^\dagger_{k_x\alpha} \left(\frac{1}{2\pi} \sum_{n_X n_x} e^{i(q_x-k_x)n_X} e^{-i(q_x+k_x)n_x/2} h^{\alpha\beta}_x \right) c_{q_x\beta} \quad \left(n_i = n_X + \frac{n_x}{2},\ n_j = n_X - \frac{n_x}{2}\right) \\
&= \int dk_x \int dq_x \sum_{\alpha\beta} c^\dagger_{k_x\alpha} \left(\delta(k_x - q_x) \sum_{n_x} e^{-ik_x n_x} h^{\alpha\beta}_x \right) c_{q_x\beta} \quad \left(\because \frac{1}{2\pi} \sum_n e^{ikn} = \delta(k)\right) \\
&= \int dk_x \sum_{\alpha\beta} c^\dagger_{k_x\alpha} \underbrace{\left(\sum_{n_x} e^{-ik_x n_x} h^{\alpha\beta}_x \right)}_{= h^{\alpha\beta}_{k_x}} c_{k_x\beta}
\end{aligned}$$

Flat-Band Limit (cont.)

By comparing the old and new Fourier transforms, one can find that (with $1/\sqrt{N} \to 1/\sqrt{(2\pi)^d}$)

$$\frac{1}{N}\sum_{\mathbf{k}} \to \int \frac{d^d k}{(2\pi)^d}$$

One may want to introduce the lattice spacing a_s into wave number k_s so that the integration over k_s is changed as

$$\int_{-\pi}^{\pi} \frac{dk_s}{2\pi} \to \int_{-\pi/a_s}^{\pi/a_s} \frac{dk_s}{2\pi/a_s}$$

which will introduce an additional factor a_s. However, in our Hall conductivity formula, the integrand contains two derivative with respect to k_s. Hence, for $d = 2$, the additional factors from the lattice spacing are canceled out. So, the integration interval is simply the Brillouin zone.

Finally, we have

$$\sigma_{xy} = \frac{e^2}{\hbar}\int_{\mathrm{BZ}} \frac{dk_x}{2\pi}\frac{dk_y}{2\pi}\sum_{\alpha=1}^{p}[F_\alpha(\mathbf{k})]_{xy} = \frac{e^2}{h}\frac{1}{2\pi}\int_{\mathrm{BZ}} dk_x dk_y \sum_{\alpha=1}^{p}[F_\alpha(\mathbf{k})]_{xy}$$

Outline

Chern Number and Quantization of Hall Conductance

- Chern number

$$\frac{1}{2\pi}\int_{\mathrm{BZ}} dk_x dk_y \sum_{\alpha=1}^{p} F_{xy}(\alpha\mathbf{k}) = (\text{integer}) \tag{112}$$

- Berry gauge field (Berry vector potential) **A** and Stokes' theorem

$$\frac{1}{2\pi}\int_{\mathrm{BZ}} dk_x dk_y\, F_{xy}(\alpha\mathbf{k}) = \frac{1}{2\pi}\int_{\mathcal{C}} d\mathbf{k}\cdot\mathbf{A}_\alpha(\mathbf{k}) \tag{113}$$

if $\mathbf{A}_\alpha(\mathbf{k})$ is well defined in the whole Brillioun zone

» Brillioun zone (2D) = a torus with no boundary

$$\int_{\mathcal{C}} d\mathbf{k}\cdot\mathbf{A}_\alpha(\mathbf{k}) = 0 \tag{114}$$

» finite values of the Berry phase $\to$ singularities of $\mathbf{A}(\mathbf{k})$ in the BZ
$=$ no global gauge that is continuous and single-valued over the entire BZ

- nonzero Chern number = obstruction to Stokes' theorem over the whole BZ

for comparison, Z_2 invariant = obstruction to Stokes' theorem in half the BZ

Chern Number and Quantization of Hall Conductance (cont.)

- observable quantities is gauge invariant, but the wavefunction and the Berry potential transform under the gauge transformation

$$|\alpha\mathbf{k}\rangle' = e^{i\zeta(\mathbf{k})}\,|\alpha\mathbf{k}\rangle \quad \text{and} \quad \mathbf{A}'_\alpha(\mathbf{k}) = \mathbf{A}_\alpha(\mathbf{k}) - \nabla_\mathbf{k}\zeta(\mathbf{k}) \tag{115}$$

- fix a smooth gauge defining a single-valued, smooth wavefunction, for example
  - » if the first component is nonzero, pick a phase to gauge-transform so that it is made real

$$|\alpha\mathbf{k}\rangle = \begin{bmatrix} a_1(\mathbf{k}) \\ a_2(\mathbf{k}) \\ \vdots \end{bmatrix} = \begin{bmatrix} |a_1(\mathbf{k})|e^{-i\zeta_1(\mathbf{k})} \\ a_2(\mathbf{k}) \\ \vdots \end{bmatrix} \to e^{i\zeta_1(\mathbf{k})} \begin{bmatrix} a_1(\mathbf{k}) \\ a_2(\mathbf{k}) \\ \vdots \end{bmatrix} = \begin{bmatrix} |a_1(\mathbf{k})| \\ e^{i\zeta_1(\mathbf{k})}a_2(\mathbf{k}) \\ \vdots \end{bmatrix} \equiv |\psi_0\rangle$$

    note that if this pick of a smooth gauge over the entire BZ is possible, the Hall conductance vanishes.
  - » failure of picking a phase when $a_1(\mathbf{k}) = 0$ at $\mathbf{k} = \mathbf{k}_i$ $(i = 1, \cdots, N_s)$
    $\to$ we define small regions (circular or of any shape) around them

$$R_i^\epsilon = \left\{\mathbf{k} \in T^2_{\mathrm{BZ}} \,|\, |\mathbf{k} - \mathbf{k}_i| < \epsilon, |\alpha\mathbf{k}_i\rangle_1 = 0\right\} \tag{116}$$

Chern Number and Quantization of Hall Conductance (cont.)

» inside R_i^ϵ, suppose that $\beta_i^{\rm th}$ component never vanishes $\rightarrow$ new choice of a gauge making $a_{\beta_i}(\mathbf{k})$ real

$$e^{i\zeta_{\beta_i}(\mathbf{k})}\begin{bmatrix}\vdots\\ a_{\beta_i}(\mathbf{k})\\ \vdots\end{bmatrix}=\begin{bmatrix}\vdots\\ |a_{\beta_i}(\mathbf{k})|\\ \vdots\end{bmatrix}\equiv|\psi_i\rangle$$

» gauge transformation between $|\psi_0\rangle$ and $|\psi_i\rangle$ at the boundary of R_i^ϵ: The gauge

$$\chi_i^\alpha(\mathbf{k})\equiv\zeta_1(\mathbf{k})-\zeta_{\beta_i}(\mathbf{k}) \tag{117}$$

defines the gauge transformation

$$|\psi_i\rangle=e^{i(\zeta_{\beta_i}(\mathbf{k})-\zeta_1(\mathbf{k}))}|\psi_0\rangle=e^{-i\chi_i^\alpha(\mathbf{k})}|\psi_0\rangle \quad \text{and} \quad \mathbf{A}_i(\mathbf{k})=\mathbf{A}_0(\mathbf{k})+\boldsymbol{\nabla}_{\mathbf{k}}\chi_i^\alpha(\mathbf{k}) \tag{118}$$

- Berry phase in terms of winding numbers

$$n_\alpha=\frac{1}{2\pi}\int_{\rm BZ}dk_xdk_y\,F_{xy}(\alpha\mathbf{k})=\frac{1}{2\pi}\sum_i\oint_{\partial(R_i^\epsilon)}d\mathbf{k}\cdot\boldsymbol{\nabla}\chi_i^\alpha(\mathbf{k}) \tag{119}$$

TI-40: proof of Eq. (119)

TI-41: prove that n_α is an integer.

Chern Number and Quantization of Hall Conductance (cont.)

TI-40: proof of Eq. (119)

Each patch has defined its smooth gauge so that the wavefunction is smoothly differentiable in it. Noting that F_{xy} is gauge-invariant, one can separate the integral into those over patches:

$$\begin{aligned}\frac{1}{2\pi}\int_{\mathrm{BZ}} dk_x dk_y\, F_{xy}(\alpha\mathbf{k}) &= \frac{1}{2\pi}\int_{T^2_{\mathrm{BZ}}-\sum_i R_i^\epsilon} dk_x dk_y\, F_{xy}(\alpha\mathbf{k}) + \sum_i \frac{1}{2\pi}\int_{R_i^\epsilon} dk_x dk_y\, F_{xy}(\alpha\mathbf{k})\\ &= \frac{1}{2\pi}\int_{T^2_{\mathrm{BZ}}-\sum_i R_i^\epsilon} d\mathbf{k}\cdot\boldsymbol{\nabla}\times\mathbf{A}_0(\mathbf{k}) + \sum_i \frac{1}{2\pi}\int_{R_i^\epsilon} d\mathbf{k}\cdot\boldsymbol{\nabla}\times\mathbf{A}_i(\mathbf{k})\end{aligned}$$

The Berry vector potentials are now well behaved in each of their respective patches, so we can apply Stokes' theorem to obtain

$$\frac{1}{2\pi}\int_{\mathrm{BZ}} dk_x dk_y\, F_{xy}(\alpha\mathbf{k}) = \frac{1}{2\pi}\int_{\partial(T^2_{\mathrm{BZ}}-\sum_i R_i^\epsilon)} d\mathbf{k}\cdot\mathbf{A}_0(\mathbf{k}) + \sum_i \frac{1}{2\pi}\int_{\partial R_i^\epsilon} d\mathbf{k}\cdot\mathbf{A}_i(\mathbf{k})$$

The torus does not have boundary, so we have $\partial(T^2_{\mathrm{BZ}} - \sum_i R_i^\epsilon) = -\sum_i \partial R_i^\epsilon$, where the minus sign means the integration in the opposite direction. Then,

$$\frac{1}{2\pi}\int_{\mathrm{BZ}} dk_x dk_y\, F_{xy}(\alpha\mathbf{k}) = \sum_i \frac{1}{2\pi}\int_{\partial R_i^\epsilon} d\mathbf{k}\cdot(\mathbf{A}_i(\mathbf{k}) - \mathbf{A}_0(\mathbf{k})) = \sum_i \frac{1}{2\pi}\int_{\partial R_i^\epsilon} d\mathbf{k}\cdot\boldsymbol{\nabla}\chi_i^\alpha(\mathbf{k})$$

Chern Number and Quantization of Hall Conductance (cont.)

TI-41: prove that n_α is an integer.

Let the boundary of the R_i^ϵ region be a perfect circle so that ∂R_i^ϵ is parameterized by

$$k = k_i + \epsilon e^{i\theta} \qquad \text{with } \theta \in [0, 2\pi)$$

Here we have used the complex representation ($z = x + iy$) for 2D wave number (k_x, k_y). Then,

$$\frac{1}{2\pi}\int_{\partial R_i^\epsilon} d\mathbf{k}\cdot\nabla\chi_i(\mathbf{k}) = \frac{1}{2\pi}\oint_{\partial R_i^\epsilon} d(\epsilon e^{i\theta})\frac{\partial\chi_i(k)}{\partial\epsilon e^{i\theta}} = \frac{1}{2\pi}\int_0^{2\pi} d\theta\,\frac{\partial\chi_i(k_i+\epsilon e^{i\theta})}{\partial\theta}$$
$$= \frac{1}{2\pi}\left(\chi_i(k_i+\epsilon e^{i(2\pi+0^-)}) - \chi_i(k_i+\epsilon)\right)$$

Since we have the single-valuedness constraint on the wavefunction,

$$|\psi_i(k_s+\epsilon)\rangle = |\psi_i(k_s+\epsilon e^{i(2\pi+0^-)})\rangle \quad \text{and} \quad |\psi_0(k_s+\epsilon)\rangle = |\psi_0(k_s+\epsilon e^{i(2\pi+0^-)})\rangle\,.$$

Since these wavefunctions are related by the gauge transformation

$$|\psi_i(k_s+\epsilon)\rangle = e^{-i\chi_i(k_s+\epsilon)}\,|\psi_0(k_s+\epsilon)\rangle$$

and

$$|\psi_i(k_s+\epsilon e^{i(2\pi+0^-)})\rangle = e^{-i\chi_i(k_s+\epsilon e^{i(2\pi+0^-)})}\,|\psi_0(k_s+\epsilon e^{i(2\pi+0^-)})\rangle\,,$$

we have

$$e^{-i\chi_i(k_s+\epsilon)} = e^{-i\chi_i(k_s+\epsilon e^{i(2\pi+0^-)})}$$

Hence, upon a full revolution around the point k_i, we necessarily have

$$\chi_i(k_s+\epsilon e^{i(2\pi+0^-)}) - \chi_i(k_s+\epsilon) = 2n\pi$$

which proves that $\frac{1}{2\pi}\int_{\partial R_i^\epsilon} d\mathbf{k}\cdot\nabla\chi_i(\mathbf{k})$ is integer.

Chern Number and Quantization of Hall Conductance (cont.)

- Hall conductance, Chern number, and winding numbers

$$\sigma_{xy} = \frac{e^2}{h} n = \frac{e^2}{h} \sum_{\alpha} n_{\alpha} \tag{120}$$

  - » the winding number n_α for band α counts the total vorticity and is gauge-invariant
    - the positions of the vorticities in the BZ can be changed, for example, by picking different components of the Bloch state to gauge-smoothen
    - the vorticities can be even separated, creating positive and negative vorticities
    - but the total vorticities are conserved
  - » Chern number is the sum of all vorticities in the BZ