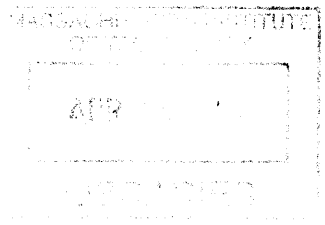

Probing the Topology in Band Insulators

by

Kuang-Ting Chen

Submitted to the Department of Physics
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Abstract

Topological Insulator is a newly found state of matter. Unlike phases described by the traditional Landau theory of symmetry breaking, the topological phases do not break symmetry, and it is not obvious in which measurable quantity will the topological index manifest itself. In this thesis, our main goal is to understand how topological classification produces measurable consequences in periodic insulators.

We first warm up by investigating the charge conjugation invariant insulator in one spatial dimension. We show there are two topological distinct classes and derive an integral formula for the topological index that distinguishes between them. We then show that the topological index appear as a Berry's phase when one adiabatically turns on a electric field.

We then study the effective theory induced by this Berry's phase and show that there are measurable consequences. We then generalize the discussion to three spatial dimensions.

It is hard to capture the topological terms in the effective theory by conventional perturbation methods. We then introduce a new formalism to calculate properties produced by those topological terms such as the polarization and the magnetization, in a unified way. The formalism is based on a perturbative expansion of the Green's functions in powers of a uniform field strength, instead of the potential. In particular, this formalism allows us to capture the effective action describing the three dimensional topological insulator defined under time reversal symmetry, which previously can only be calculated via pumping.

Finally, we discuss measurable consequences from the effective theory, in various different boundary settings. Among the properties we have calculated, we find we can identify part of them as of bulk nature, and some other part of them more as an effect associated with boundaries. For the part that are associated with boundaries, the Maxwell relation in the bulk can be violated. For example, the isotropic orbital magneto-polarizability and the orbital electric-susceptibility are different with periodic boundary conditions. However, they become identical whenever there is a boundary.

Thesis Supervisor: Patrick A. Lee
Title: Professor

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Contents

Chapter 1

Introduction

In condensed matter physics, we try to understand a phenomenon by recognizing the relevant degrees of freedom, and the interplay between them. Similar important degrees of freedom can exist in various systems independent of details of the underlying materials, and we label those systems as in the same phase. In addition to the different phases, the transitions between the phases can also possess universal properties.

Traditionally, different phases and continuous transitions between them are described by the Landau paradigm of symmetry breaking.[1] Different symmetry breaking patterns define different universality classes, where systems belonging to the same universality class share some universal properties. Many different phases and phase transitions can be understood in this way, including ferromagnets, solids, and superconductors. Generically, different ordered phase can be characterized by an order parameter which breaks certain symmetry from the disordered phase. Within the same symmetry, different states are characterized by different order parameters; usually a first-order phase transition separates between states with the same symmetry. Aside from the metallic phase which can be described in the same phase as non-interacting fermions, all other known phases fit to the description of symmetry breaking and order parameters.

In the early 1980s, the Landau paradigm is first challenged by the discovery of integer quantum Hall states.[2] By tuning the magnetic field, the integer quantum Hall system exhibits different transverse conductivity, which are quantized in units of e^2/h. These states have the same symmetry, yet the transition between them seems continuous. The symmetry breaking formulation does not give any insight into the nature of these states.

As it turns out, what separates between the integer quantum Hall states is topology.[3] Generically speaking, if the effective Hamiltonian of two insulating systems that have the same symmetry can be smoothly deformed into each other without breaking the symmetry or becoming gapless, then the two systems are in the same phase. If they cannot be deformed into each other, then they are in different phases. The effective Hamiltonian of the quantum Hall states cannot be smoothly deformed into each other without closing the energy gap. They therefore belong to different insulating phases.

Not long afer the discovery of integer quantum Hall states, people realize that there are more phases in nature that are classified by topology. Fractional Hall states[4, 5], spin liquids[6], and topological insulators[7, 8] are notable examples. Among them, the topological insulators are perhaps the simplest example, as the topology arises from the fundamental Hamiltonian, instead of some effective theory.

Unlike symmetry breaking, however, there is one important question which remains unanswered from the topological classification: how are the phases measurably different? With symmetry breaking, the symmetry itself naturally distinguishes between the phases, and the order parameter gives more detailed information. In contrast, it is not clear in general how two topologically different phases will behave in a measurably different way.

In this thesis, we are going to discuss in detail how one can probe the bulk topology for band insulators by responses to uniform electromagnetic fields. But before that, in the remaining of the chapter, I am going to review the classification of different phases as outlined above.

1.1 Landau Paradigm

Here I shall discuss two classic example of symmetry breaking: the ferromagnet and the superconductor.

1.1.1 Ferromagnet

Ferromagnetism is one of the most fascinating phenomena one can observe macroscopically at room temperature. The magnets attracts or deflects each other from a distance, depending on their orientations. There seems to be a north pole and a south pole; yet whenever one breaks a magnet into two pieces, a new pair of poles will appear.

It is thus natural to think of the ferromagnet as consisting of tiny arrows, i.e., spins, which cannot be broken into smaller parts. When those microscopic spins align, they generate macroscopic effects that we see. As one increases the temperature, at some critical temperature, the ferromagnetism disappears. Microscopically, the spins becomes disordered.

To describe the transition between the ferromagnetic phase and the disordered phase phenomenologically, one introduces the average spin variable $\hat{n}$. The free energy of the system can be written as[1]

$$F = \int \mathrm{d}^3x K(\nabla\hat{n})^2 + B\frac{(T-T_c)}{T_c}\hat{n}^2 + U(\hat{n}^2)^2; \tag{1.1}$$

with $K, B, U > 0$. If $T > T_c$, the free energy is minimized with $\hat{n}^2$=0, so that the state is disordered. If $T < T_c$, the free energy is minimized with $\hat{n}^2 = B(T_c - T)/2UT_c$, so that the average spin is not zero and point in some arbitrary direction. This breaks the rotation symmetry, and the magnitude of $\hat{n}$ is the order parameter.

Notice that in the ferromagnetic phase, the fluctuation of $\hat{n}(x)$ of momentum k carries free energy $\propto k^2$ which goes to zero in the $k \to 0$ limit. This is a physical consequence of the symmetry breaking: since changing the direction of $\hat{n}$ uniformly does not change the energy; changing $\hat{n}$ *close to uniformly* must cost little energy. In experiment, these "magnon" modes contributes a $T^{(3/2)}$ portion to the specific heat at low temperatures.

While we start from the phenomenological perspective, this effective free energy can also be derived from a microscopic Hamiltonian, say $H = \sum_{ij} -J_{ij}S_i \cdot S_j$, where S are microscopic spins and i labels individual sites. The derivation involves integrating out the high energy degrees of freedom and redefining the spins into the continuous variable $\hat{n}$. The bottom line is that one may start from various different microscopic Hamiltonians, but in the end one will end up with some effective free energy whose form only depends on the symmetry breaking pattern. In our current example, the rotation symmetry group is broken from $SO(3)$ to $SO(2)$ when the ferromagnetic moment is formed. This symmetry breaking pattern is responsible for the two magnon modes at low energies in the ferromagnetic phase.

What did we learn from this example? By thinking about the symmetry breaking between the disordered phase and the ferromagnetic phase, we gained understanding toward the universal properties of both phases and the transition between them. Have we not

thought about the symmetry breaking and focusing on the ferromagnetic state alone, we might have regarded the low energy magnons as coincidental.

1.1.2 Superconductor

In a superconductor, the free energy is given by the Ginzburg-Landau Hamiltonian[9]:

$$F = \int \mathrm{d}^3x \frac{n_s}{2m}|(\vec{\nabla} + 2ie\vec{A})\psi|^2 + \frac{B(T-T_c)}{T_c}|\psi|^2 + U|\psi|^4, \tag{1.2}$$

$\psi(x)$ is a complex field describing the superconducting amplitude, and A is the electromagnetic gauge field. Similar to the ferromagnet case, above T_c $|\psi| = 0.$ and below T_c $|\psi| = B(T_c - T)/2UT_c$, with its phase unfixed. The symmetry breaking pattern is thus $U(1)$ to nothing.

One critical difference, however, is the presence of the gauge field. The broken symmetry can be compensated by a gauge transform, which implies that the massless fluctuation in the previous case is actually a gauge fluctuation. To see this, we write $\psi = \rho e^{i\phi}$ in the superconducting phase:

$$F = \int \mathrm{d}^3x \frac{n_s}{2m}|(\vec{\nabla}\rho + (\vec{\nabla}\phi + 2ie\vec{A}))\rho|^2 + \frac{B(T-T_c)}{T_c}\rho^2 + U\rho^4, \tag{1.3}$$

one can then do a gauge transformation to absorb the ϕ dependence. From the perspective of the gauge field, the term $(4n_se^2/2m)\rho^2\vec{A}^2$ is just like a mass term. The gauge correlation in the superconductor thus is short ranged, with the correlation length inverse proportional to ρ. A static electric field or magnetic field will cost infinite energy if we keep ρ uniform, and are not allowed to exist. This is the Meissner effect.

We can also look at the current by the relation $\vec{J} = -\delta F/\delta\vec{A}$. The current is proportional to $\nabla\phi$; this implies superconductivity, as the current can exist without any electric field. Specifically, if we consider a ring of superconductor, the current flowing along the ring is *topologically* protected, due to the fact that

$$\oint \vec{\nabla}\phi \cdot \mathrm{d}\ell = 2\pi n \tag{1.4}$$

is quantized.

The superconducting amplitude $\psi(x)$ roughly describes the amplitude to annihilate two

electrons near x, with the precise spin of the electrons and their distance around x depending on the microscopics of the pairing. In the superconducting state, therefore, the electric charge is not conserved. Physically this is due to the fact that locally the superconducting ground state does not carry a definite charge. It is thus possible for two electrons to be locally absorbed into or created from the background, with the total number of electrons being conserved.

1.1.3 Quantum Phase Transitions

In the two examples above, we have discussed transitions and phases at finite temperature. These phase transitions are driven by the entropic part of the free energy. The energy favors the broken symmetry state while the entropy favors the disordered state. At zero temperature, the entropy does not contribute, and a similar phase transition is only possible when there are some other kind of competition.

One possibility is to take advantage of the non-commuting operators in quantum mechanics. For example, consider the transverse Ising model[10]

$$H = \sum_{ij} -JS_i^z S_j^z + \sum_i hS_i^x, \tag{1.5}$$

where $\vec{S}$ are Pauli matrices. Clearly, when $J >> h$, the spins formed an ferromagnet ordered in the z-direction. When $J << h$ the spins then are aligned in the x direction due to the strong magnetic field. Intuitively it is then possible to have a phase transition in between. This is called a quantum phase transition.

And from symmetry reasons, there has to be a transition: the Hamiltonian has the symmetry under the transformation $S_z \to -S_z$, $S_x \to S_x$, and $S_y \to S_y$, while the S_z ferromagnetic ground state breaks the symmetry. There must be a point in the parameter space such that $\langle S_z \rangle$ starts to be nonzero. That is the quantum critical point.

If one uses the imaginary time path integral formulation, the imaginary time integral looks a lot like another dimension of space. One can show that[10] the transverse Ising model at zero temperature is equivalent to the classical Ising model in one extra dimension. Our previous discussions are thus also useful to describe quantum phase transitions with broken symmetry as well.

To conclude this section, the Landau paradigm of symmetry breaking gives us some

information about the broken symmetry state, including an order parameter that distinguishes the state, as well as some measurable consequences. As we will see below, it is not always the case for the states that are only distinguished by topology.

1.2 Quantum Hall Effect

1.2.1 Free Electron in a Uniform Magnetic Field

In two dimensions, the electron in a uniform magnetic field is described by the following Hamiltonian if we take the Landau gauge, $A_y = Bx$:

$$H = \frac{(\vec{p} - e\vec{A})^2}{2m}. \tag{1.6}$$

Solving the Schrodinger equation, we find that in this gauge, the energy eigenstates are plane waves in the y-direction and harmonic-oscillator-like in the x-direction:

$$\psi_{nk}(\vec{x}) = e^{iky}\psi_n(x - \hbar k/eB), \tag{1.7}$$

where $\hbar k$ is the momentum in the y-direction, and $\psi_n(x)$ is the n-th energy eigenfunction of a harmonic oscillator with $\omega_0 = eB/m$. The system thus has discrete energy levels and each level contains a huge degeneracy which is only cut off by system size. These are called the Landau levels.

Now imagine we turn on an electric field in the y-direction, by changing A_y. In the adiabatic limit, the wave functions just shift their momentum in the y-direction accordingly:

$$\hbar k \to \hbar k - \frac{eEt}{\hbar}. \tag{1.8}$$

In turn, the position of each wave function shifts by

$$x \to x - \frac{E}{B}t \tag{1.9}$$

as well. The drift velocity in a magnetic field for every electron is thus given by $v_x = -\frac{E_y}{B}$,

and the total transverse current is

$$J_x = nev_x = -\frac{ne}{B}E_y, \tag{1.10}$$

which gives $\sigma_{xy} = -\frac{ne}{B}$, the same as the classical result.

However, when the chemical potential lies between two Landau levels, i.e., when the Landau levels are either completely filled or completely empty, we can treat the problem in a different way:

For concreteness let us assume the length of the sample is L in the y-direction, so that $k = 2\pi n/L$ is quantized. When we turn on A_y adiabatically, the system returns to itself with $A_y \to A_y + 2\pi\hbar/Le$. Specifically, in each Landau level, every wave function moves to the next one at the right in the same level. The charge transported in the x-direction is therefore e for every Landau level. Assuming it takes time t for the process, then we have $E_y = -2\pi\hbar/Let$ and $J_x = e/Lt$ for each occupied Landau level, which gives

$$J_x = -\frac{\nu e^2}{h}E_y; \tag{1.11}$$

ν is the number of occupied Landau levels.

This is the (integer) quantum Hall effect. As the chemical potential lies between Landau levels, the system is in an insulating phase. This only happens if there are local electron reservoir available such that the number of mobile electrons can fluctuate around to keep the chemical potential constant when the magnetic field is varied. In this case, we will observe a plateau in the transverse conductivity as a function of B.

1.2.2 Bulk-Edge Correspondence

Intuitively it is intriguing how an insulating state can possess finite transverse conductivity. In Ref. [11], Halperin pointed out that in a finite sample, the transverse current is carried by the chiral edge states on the two edges of the sample which are biased. There will be precisely one chiral edge state crossing the Fermi energy per occupied Landau level. When one biases the two edges with potential difference ΔV the occupation difference of the edge states gives precisely the transverse current $(\nu e^2/h)\Delta V$.

However, this observation does not imply the existence of an edge is a precondition for the quantum Hall effect. As we see directly from the calculation above, there is a bulk

current when one applies an electric field from the adiabatic movement of the wave functions, i.e., the "spectral flow", which occurs on the entire electron band, not only constrained to the Fermi surface. The existence of the edge states, instead of being the cause of the transverse conductivity, is a direct consequence of the spectral flow: in a finite sample, the bulk electron has to move somewhere when it flows near the edges. The only possibility is that there needs to be extra edge modes which extend from under the Fermi energy to above such that the modes flowing toward the edge can occupy.

One possible confusion is then in such finite sample, how does the Hall current distribute. Specifically, since we have both bulk current and edge current, does that not result in too much current?

The distribution of the current is determined by the gradient of the electrochemical potential. In the realistic case with edges, the electrochemical potential in the bulk is expected to be nearly a constant due to equilibrating effects. The current then is localized near the edges, and can be understood as the difference of the occupation of the edge modes. On the other hand, if we imagine a sample with periodic boundary conditions, the current will be uniformly distributed in the bulk. In either case, the total Hall current is identical and is given by $I_y = \sigma_{yx} V_x$, where V_x is the electrochemical potential difference across the entire sample.

1.2.3 Quantum Anomalous Hall Effect

The quantized transverse conductance is thus a property of an insulating state. In fact, as argued by Laughlin, the transverse conductivity has to be quantized in units of e^2/h for any phase with charge conservation and a unique ground state.[12]. The argument is similar to the spectral flow we have considered in the previous section.

In 1988, Haldane first showed a model of a periodic insulator that exhibits quantized Hall conductance in zero magnetic field[13]. The tight-binding Hamiltonian breaks time reversal symmetry. Without a magnetic field, it is straightforward to calculate the transverse conductivity via the Kubo formula:

$$\begin{aligned}\sigma_{xy}(q=0,\omega) &= \frac{ie^2}{\hbar\omega}\int \frac{\mathrm{d}^2k}{(2\pi)^2}\sum_{n\in\mathrm{occ}}\Bigg(\left\langle \psi_{nk}\left|\frac{\partial^2 H_k}{\partial k_x \partial k_y}\right|\psi_{nk}\right\rangle \\ &\quad - \sum_{m\in\mathrm{emp}}\frac{\langle\psi_{nk}|J_x|\psi_{mk}\rangle\,\langle\psi_{mk}|J_y|\psi_{nk}\rangle}{\omega-(E_m-E_n)} - \frac{\langle\psi_{nk}|J_y|\psi_{mk}\rangle\,\langle\psi_{mk}|J_x|\psi_{nk}\rangle}{\omega+(E_m-E_n)}\Bigg)\end{aligned}$$

$$\equiv \quad \sigma_{xy,P} + \sigma_{xy,D}; \tag{1.12}$$

$|\psi_{nk}\rangle$ is the Bloch state with crystal momentum k and band index n, and energy E_n, and $H_k \equiv e^{-ik\cdot\mathbf{r}} H(\mathbf{r},\mathbf{r}') e^{ik\cdot\mathbf{r}'}$ in the first quantized language. $J_x \equiv \partial H_k/\partial k_x$ and the same goes for J_y. The first term is usually called the paramagnetic current in the context of calculating the orbital magnetic susceptibility. We continue to use this notion and denote the first term $\sigma_{xy,P}$ and the second term $\sigma_{xy,D}$.

Let us from now on use the short-hand notation $|n\rangle \equiv |\psi_{nk}\rangle$ and $\partial_i \equiv \partial/\partial k_i$. Using the Feynman relation

$$\langle n\,|J_x|\,m\rangle \;= (E_n - E_m)\langle \partial_x n|m\rangle, \tag{1.13}$$

the first term can be written as

$$\begin{aligned}
\sigma_{xy,P} &= \frac{ie^2}{\hbar\omega}\int \frac{\mathrm{d}^2k}{(2\pi)^2} \sum_{n\in\mathrm{occ}} \big(-\langle \partial_y n\,|\partial_x H|\,n\rangle \;-\langle n\,|\partial_x H|\,\partial_y n\rangle \;\big) \\
&= \frac{ie^2}{\hbar\omega}\int \frac{\mathrm{d}^2k}{(2\pi)^2} \sum_{n\in\mathrm{occ},m} \big(-\langle \partial_y n|m\rangle\,\langle m\,|\partial_x H|\,n\rangle \;-\langle n\,|\partial_x H|\,m\rangle\;\langle m|\partial_y n\rangle\big) \\
&= \frac{ie^2}{\hbar\omega}\int \frac{\mathrm{d}^2k}{(2\pi)^2} \sum_{n\in\mathrm{occ},m\in\mathrm{emp}} (E_n - E_m)\big(\langle \partial_y n|m\rangle\langle \partial_x m|n\rangle + \langle \partial_x n|m\rangle\langle \partial_y m|n\rangle\big).
\end{aligned} \tag{1.14}$$

We integrate by parts in the first equality and insert a complete basis in the second. Notice that the sum over $m \in$ occ cancels using the Feynman relation, and we arrive at the last equality.

In the small ω limit, we can Taylor-expand the second term to zeroth order in ω. Using again the Feynman relation, the ω^{-1} term cancels $\sigma_{xy,P}$ exactly, as required by gauge invariance. The remaining term can be written as

$$\begin{aligned}
\sigma_{xy}(q=0,\omega\to 0) &= \frac{ie^2}{\hbar}\int \frac{\mathrm{d}^2k}{(2\pi)^2} \sum_{n\in\mathrm{occ},m\in\mathrm{emp}} \big(\langle \partial_x n|m\rangle\langle \partial_y m|n\rangle - \langle \partial_y n|m\rangle\langle \partial_x m|n\rangle\big) \\
&= \frac{-ie^2}{\hbar}\int \frac{\mathrm{d}^2k}{(2\pi)^2} \sum_{n\in\mathrm{occ}} \big(\langle \partial_x n|\partial_y n\rangle - \langle \partial_y n|\partial_x n\rangle\big) \\
&\equiv \frac{e^2}{h} C_1.
\end{aligned} \tag{1.15}$$

On first sight, the right hand side looks like a total derivative and integrates to be zero.

However, since $|\psi_{nk}\rangle$ is not required to be single-valued when one goes through the Brillouin zone, the integral needs not vanish. If we define an effective gauge field as

$$\mathcal{A}^i_{nn} \equiv -i\langle n|\partial_i n\rangle, \tag{1.16}$$

we see that the integral is the same as the field strength integrated on the Brillouin zone, which has to be an integer times 2π, by requesting that the gauge fields defined in the overlap of two patches have to be related by a gauge transform. In mathematical literature this is called the first Chern class, and in physics literature this is called the TKNN index[3]. This index is quantized, and therefore is insensitive to gradual deformation of the Hamiltonian.

We thus observe that in the quantum anomalous Hall phases, the state with different topology can be characterized by a topological index of the band structure, and the topological index is directly measured by the quantized Hall conductivity. We are interested in both the questions whether there are other topological indices that can be defined, and whether they manifest themselves in some measurable way.

1.2.4 Fractional Quantum Hall States and Topological Order

The discussion of quantum Hall effect cannot be completed without mentioning the fractional Hall states. They are however, not relevant to the topics in this thesis. I shall describe them in an intuitive manner and leave the proper introduction to Ref. [4–6]

It is quite surprising not long after the discovery of the integer quantum Hall effect, that people start to see conductivity plateaus at fractional fillings, $\nu = \frac{1}{3}, \frac{3}{7}, \frac{5}{2}, ...$, etc. These plateaus are more intricate and require cleaner sample to see. A naive analog to the integer quantum Hall analysis would suggest that the fundamental particle in those fillings carries fractional charge.

To some extent this naive picture is true. While the fundamental degrees of freedom are still electrons, strong interaction between them creates a very different ground state when the original Landau level is partially filled. In this ground state, the elementary deconfined excitations are fractional charges bound with fluxes, and they have fractional mutual statistics when one goes around another. The ground state on the torus is degenerate; when one apply the electric field to create the spectral flow, one connects one ground state to the other. These states are classified by the quasi-particle content, and the measured fractional

transverse conductance gives only partial information on the nature of the state.

More generally speaking, the fractional Hall states are examples of topological order. Another example system where we can find topological order are the spin liquids, where electrons can fractionalize into chargons and spinons which propagate independently. Generally speaking, topological order arises with strong interaction, when the defining operator of the Hamiltonian no longer provides a good description for the propagating degrees of freedom. Different topological order are distinguished by their effective theory, which contains a topological part. Even with the complication that the outer world can only communicate with the system via the defining operators, measurable responses can be found given the effective theory.

In this thesis, however, we do not deal with these systems. In a sense we are asking a more basic question. In a system where a collection of electrons is a good description, how does the topology of the Hamiltonian, in terms of bilinear electronic operators, give rise to measurable consequences? In the case of integer quantum Hall effect, the transverse conductivity is a direct measurement of the topology. Is it generally true that a topological index will give rise to some kind of quantized response?

1.3 Topological Insulator

1.3.1 Time Reversal Invariant Topological Insulators

After the discovery of the quantum anomalous Hall states, people try to come up with models that give rise to a different topological index. One simple variation is to consider the quantum anomalous Hall state as from spin-up electrons and put it together with its time reversal.[14] This way we obtain instead of the charge Hall effect, a spin Hall effect. Physically this is not so interesting however, as it is precisely the same phenomenon, with two identical copies.

It becomes more interesting when we introduce terms in the Hamiltonian that breaks S_z symmetry but leaves time reversal symmetry intact.[7] One possible term is an imaginary hopping that is proportional to S_x. With such terms, the spin current is not conserved, and the spin Hall conductance is not quantized. The original $\mathbf{Z}$ classification evaporates.

However, there is a residual $\mathbf{Z_2}$ classification, which matches to the parity of the original integer when the S_z symmetry breaking term is turned off. The easiest way to under-

stand it is via the bulk-edge correspondence: With the symmetry breaking term, counter-propagating edge modes can couple to each other. When there are an even number of edge states in each direction, everything can be gapped out. However, with an odd number, there will be one pair of edge states left. A gap cannot be formed within the two edge states due to Kramer's theorem. They will remain gapless. The $\mathbf{Z_2}$ thus distinguishes between a state with a pair of edge states on each edge, and another state without. One can also show there is a $\mathbf{Z_2}$ topological index defined in the bulk.[7, 15]

More interestingly, once we know a $\mathbf{Z_2}$ index can be defined on a 2D Brillouin zone, it is not hard to extend it to three dimensions. Consider the plane $k_z = 0$ and $k_z = \pi$ in the 3D BZ. They each carry a Z_2 index as under time reversal they are mapped into themselves. The planes in the middle can be interpreted as an interpolation between the two topologically different planar states and must break time reversal symmetry. It is apparent that interpolations between states with the same or different topology are topologically different themselves. We thus find a Z_2 index for time reversal invariant insulators in 3D as well. This is the first example of topological order in more than two dimensions.[8]

Similarly there will be surface states. We can understand as follows: suppose the surface are facing the z-direction. We parametrize the surface modes as a function of (k_x, k_y). At $k_x = 0$, the bulk system is described by the 2D BZ spanned bt (k_y, k_z). Suppose this is a topological insulator, then there must be two counter propagating gapless modes. At the Fermi energy, this gives two Fermi points on the line $k_x = 0$. Now as we shift k_x, the edge state can only disappear by gapping out each other; i.e., two Fermi points can only disappear by annihilating each other. This will happen at some $k_x < \pi$. We therefore have a closed contour as the 2D Fermi surface of the surface states.

For simplicity, let us for now think of the eigenstate as living on the Bloch sphere. The surface state at (k_x, k_y) is the time reversal of the state at $(-k_x, -k_y)$, and they are at the opposite poles on the Bloch sphere. When we go around the Fermi surface, the solid angle swept by the contour on the Bloch sphere then is restricted to be 2π, which gives a Berry's phase of π. As we change the chemical potential, the Berry's phase cannot be changed until the Fermi surface shrinks to a point, where it is doubly degenerate. Through the point the Berry's phase jump by 2π, as the rotation of the eigenstate on the Bloch sphere reverses its direction. This is because two eigenstates at the same momentum have to be orthogonal. Tracing out the Fermi surface across the energy, we find the surface state is described by a

single Dirac cone.

The signature of the time reversal invariant topological insulators is thus the existence of an odd number of pairs of edge states in 2D, or Dirac cones in 3D. On the other hand, since the topological index is defined in the bulk, intuitively one might expect there are also bulk signatures that distinguishes between the states, similar to the quantized transverse conductivity of the quantum anomalous Hall states. This is the key question we are going to address in this thesis.

1.3.2 Effective Action and Dimensional Reduction

We are not among the first trying to think about topological responses in the bulk. In 2008, Qi et. al.[16] tried to identify the topological insulators by possible topological terms in the electromagnetic effective action. In two spatial dimensions, the Chern-Simons term in spacetime describes precisely the transverse conductivity. In general, in even spatial dimensions, there is a Chern-Simons like term

$$S_{2d} \propto \int \mathrm{d}^{2d}x\ \mathrm{d}t\epsilon^{i_1 i_2 \cdots i_{2d+1}} A_{i_1} F_{i_2 i_3} ... F_{i_{2d} i_{2d+1}} \tag{1.17}$$

which is topological and produces transverse responses when electromagnetic fields are applied in all the remaining directions. In odd spatial dimensions, there is a total derivative term

$$S_{2d+1} \propto \int \mathrm{d}^{2d-1}x\ \mathrm{d}t\epsilon^{i_1 i_2 \cdots i_{2d}} F_{i_1 i_2} ... F_{i_{2d-1} i_{2d}} \tag{1.18}$$

which does not alter the equation of motion. We can also see the bulk integral of S_{2d+1} is the same as S_{2d} integrated on the boundary.

Starting in four spatial dimensions, they show that integrating out the band electrons results in a quantized coefficient C_2 in front of S_4. Furthermore, the coefficient C_2 is the second Chern number defined from the nonabelian Berry's phase gauge field $\mathcal{A}_{\mu,nn'}$:

$$C_2 \propto \int \mathrm{d}^4 k \epsilon^{\mu\nu\lambda\sigma} \mathrm{tr}\big(\mathcal{F}_{\mu\nu}\mathcal{F}_{\lambda\sigma}\big); \tag{1.19}$$

$$\mathcal{F}_{\mu\nu} \equiv \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu - i[\mathcal{A}_\mu, \mathcal{A}_\nu]; \tag{1.20}$$

$$\mathcal{A}_{\mu,nn'} \equiv \langle u_{nk}| - i\frac{\partial}{\partial k^\mu}|u_{n'k}\rangle. \tag{1.21}$$

Similar to the previous subsection, we can treat the 4d Hamiltonian as a series of 3d Hamiltonians, say as a function of k_u. In order to have the response described by S_{4d}, say, a current in the x direction with the magnetic field in the $x-y$ plane and an electric field in the u direction, each slice of 3d Hamiltonian needs to respond to B_{xy}, when the Hamiltonian changes with time:

$$J_x = \int \mathrm{d}k^u \partial_t \theta(H_{3d}(k_u)) B_{xy} = \int \mathrm{d}k_u \partial_u \theta(H_{3d}(k_u)) B_{xy} E_u \propto C_2 B_{xy} E_u. \tag{1.22}$$

Here θ is some function of H_{3d}, which gives the response to B_{xy} when H_{3d} is varied with time. We then see that

$$C_2 \propto \int \mathrm{d}k^u \partial_u \theta; \tag{1.23}$$

in other words, C_2 measures the winding of θ, when one goes across the Brillouin zone. For C_2 to possibly be nonzero, θ cannot be a single-valued function of H_{3d}. ($\partial_u \theta$, however, is a single valued function of H_{3d} since it describes a current response. This is similar to the angular variable and the angular velocity.) In fact, from the expression of C_2, we can write θ as

$$\theta(H_{3d}) \propto \int \mathrm{d}^3 k \epsilon^{ijk} \mathrm{tr}(\mathcal{A}_i \partial_j \mathcal{A}_k - i\frac{2}{3} \mathcal{A}_i \mathcal{A}_j \mathcal{A}_k) + F(H_{3d}); \tag{1.24}$$

F is an arbitrary single valued function.

The effective action of H_{3d} can be written down to give rise to the current. Up to a total derivative, we have:

$$\begin{aligned} S_{3d} &\propto \int \mathrm{d}^3 x \mathrm{d}t \; A_i J_i \\ &\propto \int \mathrm{d}^3 x \mathrm{d}t \; \partial_t \theta \epsilon^{ijk} A_i F_{jk} \\ &\propto \int \mathrm{d}^3 x \mathrm{d}t \; \theta \epsilon^{\mu\nu\lambda\sigma} F_{\mu\nu} F_{\lambda\sigma}. \end{aligned} \tag{1.25}$$

Therefore, the required effective action in 3d to give rise to the transverse current in 4d is exactly the topological term in 3d. Notice that θ is odd under time reversal; with the understanding that θ is not single valued like an angle, it can take either 0 or π with proper normalization, when time reversal symmetry is conserved. $\theta = 0$ describes the trivial insulator, while $\theta = \pi$ describes the topological insulator. It is shown in Ref. [17] that this distinction is exactly the same as the two different states discussed in the previous section.

Notice that S_{3d} describes the response when the Hamiltonian is adiabatically varied. It thus gives the current discussed above, as well as an edge quantum Hall effect when the time reversal symmetry is locally broken on the edge and the Hamiltonian smoothly change from the topological one to the trivial one. In Ref. [18] it is pointed out that the edge quanum Hall effect gives rise to a bulk magneto-electric effect.

When time reversal symmetry conserved, θ can readily be calculated by the formula

$$\theta(H_{3d}) \propto \int \mathrm{d}^3k\epsilon^{ijk}\mathrm{tr}(\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k). \tag{1.26}$$

This is because a single-valued, time-reversal-odd function must vanish when time reversal symmetry is present; we therefore can set $F = 0$.

However, one thing that is not completely clear from the discussion is whether S_{3d} gives any physical effect when the Hamiltonian is not varied either as a function of space or time. In this thesis we are going to clarify this issue. Another complication is that we might be interested in the general situation, when time reversal symmetry is broken. The discussion above does not constrain S_3d enough to derive the general formula of θ, as well as other possible non-topological terms. Ref. [19] derived the general formula of θ as well as the accompanied off-diagonal non-topological responses by considering a general pumping process in a magnetic field. In this thesis, we are going to derive the same formula in a more systematic way without pumping.

With an effective theory description of the 3d topological insulator, one might wonder about the 2d topological insulator. The same discussion is not applicable to one lower dimension however, due to the fact that S_3d is already a total derivative, and does not require the effective action S_{2d} to be of any specific form.

1.3.3 Topological Classification of Non-interacting Gapped Systems

Here we briefly discuss the general classification scheme of noninteracting insulators that preserves various symmetries. Not long after the discovery of the 2d and 3d topological insulators, people realize that similar classification is possible also for superconductors. This is because at mean-field level, a superconductor is just like an insulator, but with particle-hole symmetry.

There are two approaches to the problem: Kitaev considered classifying the Hamiltonian

complex case:

Cartan\d	0	1	2	3	4	5	6	7	8	9	10	11	$\cdots$
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$

real case:

Cartan\d	0	1	2	3	4	5	6	7	8	9	10	11	$\cdots$
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\cdots$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\cdots$
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	$\cdots$
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\cdots$
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\cdots$
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\cdots$
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\cdots$
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	$\cdots$

Table 1.1: Classification of topological insulators and superconductors as a function of spatial dimension d and symmetry class, indicated by the "Cartan label" (first column). This table is reproduced from Ref. [21].

in arbitrary spatial dimensions with translational symmetry, in addition to either particle-hole symmetry or time reversal symmetry.[20] The corresponding mathematical theory is called twisted K-theory. Another approach is to take advantage of the bulk-edge correspondence and study the edge states. Ryu et. al. study the localization properties of the edge Hamiltonian and obtain the same result, as shown in the following table:[21]:

Depending on the symmetry, the classification is periodic in the spatial dimension with period two or eight.

1.4 Outline

In this thesis, we are going to focus on the problem how the topology of a band insulator give rise to measurable properties in the bulk, without varying the Hamiltonian. We are going to show that the polarization and the magnetization contains topological information, and devise a systematic way to calculate them. We will also discuss the dependence of the bulk properties on boundary conditions. The chapters are organized as follows:

In chapter two, we consider the charge-conjugation invariant topological insulator in 1d to illustrate how states are topologically different under a symmetry, and how the topological index can be expressed either in a discrete or integral form. We will also see how the

topological index appear in the effective action.

In chapter three, we consider the physical consequence having the topological term in one and three dimensions, without a boundary.

In chapter four, we switch back and consider the possibility to derive the effective action in a more conventional perturbation theory. We will describe and explain the difficulty we encounter in this approach.

In chapter five, we develop a Green's function formalism, perturbative in orders of the external field strength, instead of the potential. We then use this formalism to calculate various effective actions with periodic boundary conditions.

In chapter six, we will investigate how the presence of a boundary can alter the physics. We will conclude in chapter seven.

Chapter 2

A Case Study: Charge Conjugation Invariant Insulators in 1d

In this chapter, we discuss the topological insulator in one spatial dimensions defined under charge conjugation symmetry in detail. We first see explicitly how the two classes of insulators are topologically different, and then we will see how this difference show up when coupled to an external electric field.

2.1 Topology of Charge Conjugation Invariant Gapped Hamiltonians in Zero Spatial Dimensions

Charge conjugation is defined by the an antiunitary operation $\mathbf{C}$ with the constraint $\mathbf{C}^2 = 1$.[16] If we write $\mathbf{C} = CK$, where K is complex conjugation and C is an unitary matrix, the condition $\mathbf{C}^2 = 1$ leads to $CC^* = 1$. A charge conjugation invariant (CCI) Hamiltonian H is defined such that if a state $|\psi\rangle$ is of energy E, then $\mathbf{C}|\psi\rangle$ is of energy $-E$. This translates to the condition

$$HC = -CH^*. \tag{2.1}$$

In this section, we want to show that the space of CCI Hamiltonians with a gap contains two disjoint subset which cannot be smoothly deform into each other. In other words, in zero dimensions there is a $\mathbf{Z}_2$ classification.

Consider one CCI Hamiltonian h with $2n$ bands. First we deform h so that the occupied bands are of energy eigenvalue -1 and the empty bands are of eigenvalue $+1$. Now we can

choose the eigenbasis of h, such that C is in the form

$$C = \begin{pmatrix} \mathbf{0} & \mathbf{1}_n \\ \mathbf{1}_n & \mathbf{0} \end{pmatrix}, \tag{2.2}$$

which satisfies $CC^* = 1$ and $CC^\dagger = 1$. In this basis, the space of all CCI Hamiltonians can be expressed as

$$h \in \{Sh_0S^\dagger, (SS^\dagger = 1) \wedge (hC = -Ch^*)\}, \tag{2.3}$$

where

$$h_0 = \begin{pmatrix} \mathbf{1}_n & \mathbf{0} \\ \mathbf{0} & -\mathbf{1}_n \end{pmatrix}. \tag{2.4}$$

In other words, the topology of h is contained in the topology of the eigenbasis S, which are $2n$ by $2n$ complex matrices satisfying $SS^\dagger = 1$ and $S^\dagger CS^* = C$; the latter condition comes from the charge-conjugation invariance of h. With C being real, the condition can also be written as $S^T CS = C$.

Now let us perform a real orthogonal transformation to make C diagonal:

$$C' = \Lambda C \Lambda^T = \begin{pmatrix} \mathbf{1}_n & \mathbf{0} \\ \mathbf{0} & -\mathbf{1}_n. \end{pmatrix} \tag{2.5}$$

We also have $S' \equiv \Lambda S \Lambda^T$ in this basis. Let $S' = X + iY$ where X and Y are both real. Pluging in the condition $S^T CS = C$ and $S^\dagger S = SS^\dagger = 1$, we can show that X and Y must be in the form

$$X = \begin{pmatrix} X_{11} & \mathbf{0} \\ \mathbf{0} & X_{22} \end{pmatrix}, \; Y = \begin{pmatrix} \mathbf{0} & Y_{12} \\ Y_{21} & \mathbf{0} \end{pmatrix}, \tag{2.6}$$

with the conditions

$$\begin{aligned} X_{11}^T X_{11} + Y_{21}^T Y_{21} &= \mathbf{1}_n, \\ X_{22}^T X_{22} + Y_{12}^T Y_{12} &= \mathbf{1}_n, \\ X_{11} X_{11}^T + Y_{12} Y_{12}^T &= \mathbf{1}_n, \\ X_{22} X_{22}^T + Y_{21} Y_{21}^T &= \mathbf{1}_n, \\ X_{11}^T Y_{12} - Y_{21}^T X_{22} &= \mathbf{0} \end{aligned}$$

$$X_{11}Y_{21}^T - Y_{12}X_{22}^T = \mathbf{0}. \tag{2.7}$$

To show that the space contains two disconnected pieces, we will show in the following that the sign of $\det X$ cannot change, under smooth changes that obey the conditions above.

In order for $\det X$ to change sign, it has to go through zero. At least one of the *singular values* of X thus has to be small during the process. Without loss of generality, let us consider X_{11} has a small singular value ϵ with the corresponding right singular vector $|u_1(\epsilon)\rangle$ and left singular vector $|v_1(\epsilon)\rangle$:

$$\begin{aligned} X_{11}|u_1(\epsilon)\rangle &= \epsilon|v_1(\epsilon)\rangle; \\ X_{11}^T|v_1(\epsilon)\rangle &= \epsilon|u_1(\epsilon)\rangle. \end{aligned} \tag{2.8}$$

By the first constraint, $|u_1(\epsilon)\rangle$ is also a singular vector of Y_{21} to first order in ϵ:

$$Y_{21}^T Y_{21}|u_1(\epsilon)\rangle = |u_1(\epsilon)\rangle + O(\epsilon^2); \tag{2.9}$$

Now we apply the fifth constraint on $\langle u_1(\epsilon)|$. We get

$$\langle u_1(\epsilon)|Y_{21}^T X_{22} \sim O(\epsilon). \tag{2.10}$$

Since $|u_1(\epsilon)\rangle$ is a singular vector of Y_{21} with singular value ~ 1, X_{22} must also have an singular value of order $O(\epsilon)$. Let us denote the singular value as δ:

$$\begin{aligned} X_{22}|u_2(\epsilon)\rangle &= \delta|v_2(\epsilon)\rangle; \\ X_{22}^T|v_2(\epsilon)\rangle &= \delta|u_2(\epsilon)\rangle. \end{aligned} \tag{2.11}$$

Now let us take advantage of the first four constraints. Similar to above, we can deduce from the fourth constraint that the left singular vector of Y_{21} with singular value ~ 1 is just $|v_2(\epsilon)\rangle$. Similarly, Y_{12} has to have a singular value ~ 1 with left singular vector $|v_1(\epsilon)\rangle$, and right singular vector $|u_2(\epsilon)\rangle$.

Now we can take the matrix element of the last equality between $|v_2(\epsilon)\rangle$ and $\langle v_1(\epsilon)|$. (Taking the second-to-last equation between the u's will yeild identical result.) Using all

the singular values and singular vectors, up to $O(\epsilon)$ we have

$$\delta - \epsilon = 0. \tag{2.12}$$

Therefore, when we gradually deform one of the singular value of X to be zero, there will be another one that is going to be zero at the same time. Furthermore, the two singular values are equal to each other when they are small. The determinant of X, being the product of the singular values, thus do not change sign.

When multiple singular values are approaching zero at the same time, by the same analysis they have to come in pairs. Within each pair the product of the singular values does not change sign. $\det(X)$ therefore cannot change sign under arbitrary deformation of h that respects charge-conjugation symmetry.

How do we understand such two disjoint pieces of CCI Hamiltonians? Let us consider a deformation S which exchanges one occupied band with one empty band:

$$S = \sigma_x \bigoplus \mathbf{1}_{2n-2}. \tag{2.13}$$

We then have $\det(X) = -1$. For a trivial deformation $S = \mathbf{1}_{2n}$ $\det(X) = 1$. The two disjoint part of the space of CCI Hamiltonians can thus be represented by some Hamiltonian, and another Hamiltonian which results from exchanging an odd number of bands from being occupied to empty and vice versa.

One can also see this intuitively. Suppose we want to smoothly exchange $|u\rangle$ and $|v\rangle$ without touching other energy eigenstates. Apparently $|u\rangle$ and $|v\rangle$ have to be charge conjugate pairs for the exchange to be charge conjugation invariant. We can take the phase definition of the vectors such that $|u\rangle \to |v\rangle$ and $|v\rangle \to |u\rangle$ under charge conjugation. Let us parametrize the transformation:

$$\begin{aligned} |u\rangle' &= \cos\theta|u\rangle + \sin\theta e^{i\phi}|v\rangle; \\ |v\rangle' &= \cos\theta|v\rangle - \sin\theta e^{-i\phi}|u\rangle. \end{aligned} \tag{2.14}$$

The transformation has to be of this form in order to keep $|u\rangle'$ and $|v\rangle'$ orthogonal. But now we can see that $|u\rangle'$ does not transform to $|v\rangle'$ under charge conjugation, due to the sign in front of $\sin\theta$!

On the other hand, if we smoothly exchange two pairs of charge conjugation pairs the problem disappears. Suppose we have $|u_1\rangle$, $|v_1\rangle$, $|u_2\rangle$, and $|v_2\rangle$, where u's and v's are charge conjugate pairs. The transform described by

$$\begin{aligned} |u_1\rangle' &= \cos\theta|u_1\rangle + \sin\theta e^{i\phi}|v_2\rangle; \\ |v_1\rangle' &= \cos\theta|v_1\rangle + \sin\theta e^{-i\phi}|u_2\rangle; \\ |u_2\rangle' &= \cos\theta|u_2\rangle - \sin\theta e^{i\phi}|v_1\rangle; \\ |v_2\rangle' &= \cos\theta|v_2\rangle - \sin\theta e^{-i\phi}|u_1\rangle \end{aligned} \tag{2.15}$$

has no problem being both orthogonal and charge conjugation invariant.

We have thus understood that the CCI Hamiltonian in zero dimensions is classified by $\mathbf{Z}_2$. However, We note that even though the two sets of Hamiltonians are disconnected, there are no physical distinction, and a global relabelling of the basis transform the two classes to each other.

2.2 The Classification of Charge Conjugation Invariant Insulators in One Dimension

The simplest way to define the Hamiltonian in various dimensions of space is to assume translation symmetry. The Hamiltonian then has eigenvalues and eigenvectors labeled by the crystal momentum k, which we take to have a range of $[-\pi, \pi)$. In the case we are interested, the Hamiltonian is non-interacting, and can be decomposed in to a sum of the Hamiltonians at different k. For a system with $2n$ bands, the Hamiltonian $H(k)$ is then a $2n \times 2n$ matrix at each k. Under charge conjugation symmetry, we require the Hamiltonian to satisfy the following constraint:

$$H(k)C = -CH^*(-k); \tag{2.16}$$

physically, a local charge conjugation operation also flips the momentum.

While the Hamiltonian at some given k do not have any constraint (except being related to the Hamiltonian at $-k$ by the condition above), at $k = 0$ and $k = \pi$, we must have 0d CCI insulators, due to the fact that the momenta are mapped to themselves. Since there are two

disjoint set of 0d CCI gapped Hamiltonians (calling them + and −), the 1d CCI insulator is labeled by the CCI Hamiltonians at those momentum: if we use the pair $(\cdots,\cdots)$ to label the Hamiltonian at $k = 0$ and $k = \pi$ respectively, $(++)$, $(--)$, $(+-)$, and $(-+)$ are the four possibilities.

However, while + and − are distinct, they are not physically different. Interestingly, for the 1d CCI insulator, we can find two classes out of the four, which are physically different: the *trivial* one interpolates between two gapped CCI Hamiltonians in the same class while the *topological* one interpolates between different classes. The topological classification of 1d CCI insulators is thus $\mathbf{Z}_2$ once we allow global redefinition of the basis. We can define a topological index which is just the multiplication of the two 0d $\mathbf{Z}_2$ indices at $k = 0$ and $k = \pi$.

Before closing, let us mention in general how this procedure can generalize to higher dimensions. Naively it seems that we can then obtain a $\mathbf{Z}_2$ classification for 2d CCI insulators as well, with two additional $\mathbf{Z}_2$s that are of 1d nature, describing the topology of the line $k_x = 0$ and $k_y = 0$ in the Brillouin zone.

This turns out not to be correct, due to the fact that the classification obtained this way is not necessarily complete. In fact, the quantum Hall effect does not necessarily break charge conjugation, and 2d CCI insulators are classified by $\mathbf{Z}$. The $\mathbf{Z}_2$ obtained is just the parity of the $\mathbf{Z}$.

If we consider further, building from 2d to 3d, we face another difficulty. We have thus far assumed that it is possible to interpolate between different CCI insulaters if we break the charge conjugation symmetry. However, as we know, an interpolation between different quantum Hall states is just impossible without closing the gap. Therefore, there are no intrinsic topological classification for CCI insulators in 3d.

2.3 Integral Form of the Topological Index

Turning back to 1d, let us consider the following integral:

$$P = \frac{-i}{2\pi}\int_{-\pi}^{\pi} \sum_{\alpha(k)\in occ} \langle\alpha(k)|\frac{\partial}{\partial k}|\alpha(k)\rangle \mathrm{d}k; \tag{2.17}$$

$|\alpha(k)\rangle$ denotes the periodic part of the Block eigenstates with crystal momentum k. For an insulator, this integral is in sensitive to the small "gauge transformation" by $|\alpha(k)\rangle \to e^{i\phi(k)}|\alpha(k)\rangle$ where $\phi(k)$ is a small number. The integral can shift by an arbitrary integer when $\phi(k)$ is large and wind around when we go across the Brillouin zone, however; therefore, P is only defined modulo 1. With these properties in mind, let us evaluate the integral using the charge conjugation symmetry:

$$\begin{aligned} P &= \frac{-i}{2\pi}\int_{-\pi}^{0}\sum_{\alpha(k)\in occ}\langle\alpha(k)|\frac{\partial}{\partial k}|\alpha(k)\rangle \mathrm{d}k \\ &+\frac{-i}{2\pi}\int_{0}^{\pi}\sum_{\beta(-k)\notin occ}\langle\beta(-k)|K^\dagger C^\dagger\frac{\partial}{\partial k}CK|\beta(-k)\rangle \mathrm{d}k. \end{aligned} \tag{2.18}$$

We express the occupied states within $k \in (0,\pi)$ by the unoccupied states at $k \in (-\pi, 0)$ using the charge-conjugation symmetry. Noting that $C^\dagger C = 1$, and using the fact that

$$\langle v|K^\dagger K|u\rangle = \langle u|v\rangle, \tag{2.19}$$

we can rearrange the second term and combine:

$$P = \frac{-i}{2\pi}\int_{-\pi}^{0}\sum_{\alpha}\langle\alpha|\frac{\partial}{\partial k}|\alpha\rangle \mathrm{d}k, \tag{2.20}$$

where $|\alpha\rangle$ now runs over all states.

Let us consider first if at $k = 0$ and $k = \pi$ the Hamiltonians are in the same class. Let us consider an auxiliary CCI Hamiltonian $H'(k)$, where at $k = \pm k'$ we have $H'(k) = H(0)$. For k in the range $-\pi < k < -k'$ and $k' < k < \pi$, we have $H'(k) = H(\pi k/(\pi - k'))$; i.e., the auxiliary Hamiltonian is changing in the same way as the original Hamiltonian. For $-k' < k < k'$, we let H' vary in some charge conjugation invariant way from $H(\pi)$ to $H(0)$, so that $H'(0) = H(\pi)$ and $H(k) = H(-k)$.

Evidently we have

$$\frac{-i}{2\pi}\int_{-\pi}^{0}\sum_{\alpha(H)}\langle\alpha(H)|\frac{\partial}{\partial k}|\alpha(H)\rangle \mathrm{d}k = \frac{-i}{2\pi}\int_{-\pi}^{-k'}\sum_{\alpha(H')}\langle\alpha(H')|\frac{\partial}{\partial k}|\alpha(H')\rangle \mathrm{d}k. \tag{2.21}$$

In addition, the integral over the range $-k' < k < 0$ vanishes for H':

$$\begin{aligned}
&\int_{-k'}^{0} \sum_{\alpha(H')} \langle \alpha(H') | \frac{\partial}{\partial k} | \alpha(H') \rangle \mathrm{d}k \\
= &\int_{-k'}^{0} \sum_{\alpha(H') \in occ} \langle \alpha(H') | \frac{\partial}{\partial k} | \alpha(H') \rangle + \int_{-k'}^{0} \sum_{\alpha(H') \in emp} \langle \alpha(H') | \frac{\partial}{\partial k} | \alpha(H') \rangle \\
= &\int_{-k'}^{0} \sum_{\alpha(H') \in occ} \langle \alpha(H') | \frac{\partial}{\partial k} | \alpha(H') \rangle - \int_{-k'}^{0} \sum_{\alpha(H') \in occ} \langle \alpha(H') | \frac{\partial}{\partial k} | \alpha(H') \rangle \\
= &\ 0. \qquad (2.22)
\end{aligned}$$

The second equality similarly follows from Eq. (2.19). We therefore have

$$P(H) = P(H'). \qquad (2.23)$$

Notice that $P(H')$ is a loop integral, which has to be an integer. We therefore have shown that for the trivial CCI insulator, P has to be an integer.

On the other hand, if the Hamiltonians at $k = 0$ and $k = \pi$ are in different classes, the same procedure does not apply. The interpolation within $-k' < k < k'$ has to break charge conjugation symmetry. However, the integral of any such two Hamiltonians can be joined to form a loop integral, which then has to take integer values. The only consistent value for the integral of a single Hamiltonian is then a half integer. We conclude that P has to be a half integer for the topological CCI insulator. P is thus a topological index in integral form that distinguishes the two classes of CCI insulators in one dimension.

2.4 Topological Index as a Berry's phase

In the discrete form, it is hard to see how the topological index can be probed. In order to probe the Hamiltonians at $k = 0$ and $k = \pi$, one needs some kind of perturbation which couples the two together. A phonon or photon with momentum π can do the job, but then they couple to all electron pairs that have a momentum difference of π. The heart of the problem is that while $k = 0$ and $k = \pi$ are special, invariant momentum under charge conjugation, this speciality does not carry over to the way they are coupled with external perturbations.

The integral form of the topological index is more accessible, simply due to the fact that

the formula contains a momentum space integral which treat all momentum on the same footing. Interestingly, from the form of the integral we realize that we should expect some $q = 0$ effect from the topological index instead of $q = \pi$, as now the integrand involves states only at the same momentum. We will see in the following, that the topological index emerges as a Berry's phase when one turns on the electric field.

If we think about effective action for an energy eigenstate, it just describes a phase that is accumulated with time. For an insulator this observation is particularly useful, as physically we expect the insulator is indeed an energy eigenstate that almost does not change in the presence of the external field.

Technically, in an insulator, this phase should be calculated by integrating out the fermions in a time-dependent back ground field. Physically the phase has two distinct contributions though: one can be understood as the time-dependent energy of the fermions, and the other is a Berry's phase of the process, defined only when the fermions going back to the original state. The phase shift from the energy depends on the time duration and is not just a function of the initial and final state, whereas the Berry's phase depends only on the trajectory in the Hilbert space.

Let us focus on the Berry's phase part. Similar to the consideration in Ref.[22, 23], let us consider the accumulated geometric phase of the band electrons, when the external field is slowly turned on:

Let us take the temporal gauge. First we shall consider how the single particle wave function change as we increase the gauge field A_1 uniformly. We have

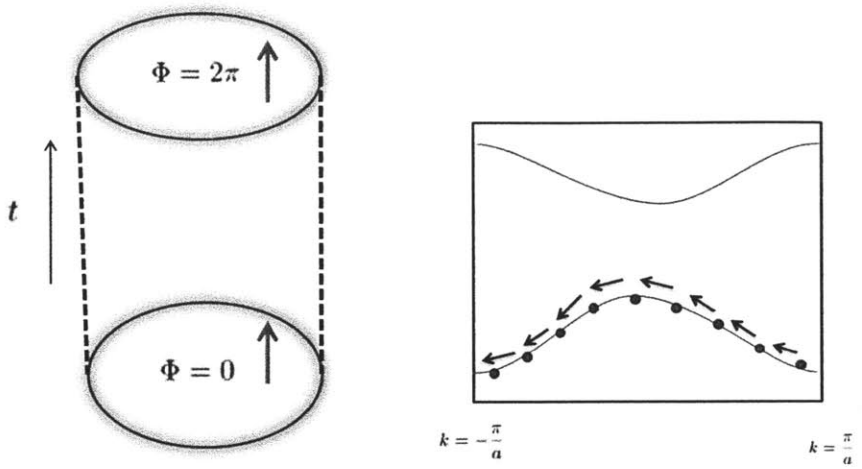
$$\psi_{nk}(x) = u_{nk}(x)e^{ikx} \tag{2.24}$$

which is the wave function in position basis, and $u_{nk}(x)$ is periodic and satisfies

$$\left((\nabla - (k + eA_1))^2 + V(x)\right) u_{nk}(x) = E_{nk}u_{nk}(x). \tag{2.25}$$

As we increase A_1 uniformly to $A_1 + \eta$, the momentum k cannot change as it is fixed by the finite size L and the periodic boundary condition. On the other hand, following Eq. (5.14), $u_{nk}(x)$ changes as

$$u_{nk}(A_1 + \eta) = u_{n(k-e\eta)}(A_1), \tag{2.26}$$



(a) the procedure (b) spectral flow

Figure 2-1: (a) A flux is slowly threaded through. $\Phi = 0$ and $\Phi = 2\pi$ are the same physical state related by a gauge transform. We calculate the Berry's phase of the process. (b) During the process, at every allowed momentum by the periodic boundary conditions, the energy and the periodic part of the wave function moves slowly to the values of the state to the left, according to Eq. (5.15). When a full flux is threaded, each one of them takes the eigenvalue and the eigenvecotor of the one at its left. Note that the momentum quantum number k, however, does not change. When we sum over the Berry's phase contribution from all the single particle states, it becomes an integral over the entire Brillouin zone.

which is just a corresponding shift of k by $-e\eta$. if $e\eta = 2\pi/L$, the system returns to its original state, but in a different gauge (i.e., with winding number different by one.) Notice that while $u_{nk}(x)$ goes to the next avaiable value on the left, the k in the exponential stays the same. The electronic wave function is therefore different from its starting state. Nevertheless, as discussed further below, if we include the gauge field, the final state differs from the initial state by a large gauge transformation, and the Berry's phase accumulated in the process is exactly what we want to calculate.

As a side note, the situation is similar if we put electrons on a lattice which couples to the gauge field via Periels substitution. The single particle eigenfunction can be written as $\psi_{nk} = \sum_i u_{nk,m} \exp(ikx_i)|m, x_i\rangle$, with u_{nk} now a vector in the orbital space. With an increase of A_1, only u_{nk} changes.

Now we are ready to calculate the accumulated Berry's phase of the band electrons

under the process, where the winding of the gauge field is increased by one:

$$\begin{aligned}
\phi_{\text{Berry}} &= i\int_{2\pi n/e}^{2\pi(n+1)/e} \mathrm{d}\tilde{\mathrm{A}}_1(0)\langle\Psi_{\mathrm{e}}|\frac{\partial}{\partial\tilde{\mathrm{A}}_1(0)}|\Psi_{\mathrm{e}}\rangle \\
&= i\int_{2\pi n/e}^{2\pi(n+1)/e} \mathrm{d}\tilde{\mathrm{A}}_1(0)\sum_{\mathrm{k_i},\alpha\in\mathrm{occ}}\langle\psi_{\mathrm{k_i}\alpha}|\frac{\partial}{\partial\tilde{\mathrm{A}}_1(0)}|\psi_{\mathrm{k_i}\alpha}\rangle \\
&= i\sum_{k_i,\alpha\in\mathrm{occ}}\int_{k_i}^{k_i+2\pi/L}\mathrm{d}k\langle u_{k\alpha}|\frac{\partial}{\partial k}|u_{k\alpha}\rangle \\
&= i\int_{\mathrm{BZ}}\mathrm{d}k\sum_{\alpha\in\mathrm{occ}}\langle u_{\alpha k}|\frac{\partial}{\partial k}|u_{\alpha k}\rangle \\
&= -2\pi P. \qquad (2.27)
\end{aligned}$$

In the second equality, we wrote the derivative acting on the Slater determinent as a sum of derivatives acting on single particle wave functions. In the third equality we then plug in the dependence of the wave functions, and change variables to k. Whenever $\tilde{A}_1(0)$ increases by $2\pi/e$, each u_{nk} reaches the next allowed eigenstate to the left by the periodic boundary condition (without actually changing the momentum eigenvalue.) As we sum over all the integral of eigenstates at different allowed k's, the whole Brillouin zone (BZ) is covered exactly once and we reach the fourth equality.

While we calculate the Berry's phase for process where the winding number of the initial and final states differs by one, evidently the phase is proportional to the difference of the winding number in general, which is just the spacetime integral of the electric field. Therefore, in the effective action, a term $\int \mathrm{d}x\mathrm{d}t\ (-P\cdot E)$ appears. We thus have showed that the topological index we find to distinguish between topological distinct CCI insulators appear directly in the effective theory of the external fields. In addition, the term $(-P\cdot E)$ is just the topological term (θ term) we have discussed in Sec. 1.3.2. Also, since P couples linearly to the electric field it is also understood as the ground state polarization. The same formula was derived in Refs. [23, 31].

A few remarks are in order. First, this calculation is good for a finite-size system, where both the lattice spacing and the length of space are finite. Despite that the eigenstates in such a system would be discrete points in the BZ, the whole BZ is covered by the integral and there is no finite-size effect. Second, one might notice that the fermionic wave functions of the initial and final state are different, and it seems that our process does not form a close loop as usually required by a physical (gauge-invariant) Berry's phase. This does not

invalidate our calculation, however, since the initial state and the final state are related by a large gauge transform. There are however subtleties which we shall investigate after we understand the physical consequence of having this Berry's phase.

We have thus showed in one spatial dimensions, how the the band structures invariant under charge conjugation are topologically distinct. We developed an integral formula for the topological index, which distinguishes between the two classes. We then showed how this topological index appear as a Berry's phase when one gradually turns on the electric field. This Berry's phase naturally appears as the topological term (θ term) in the effective theory in one spatial dimension.

In the subsequent chapters, I will first discuss the consequence of the topological term in various dimensions. I will then develop a framework to generalize the Berry's phase calculation here to higher dimensions, which is not constrained to linear order for the coupling to the external fields. I will not, however, prove the classification or derive the topological index that distinguishes them as I have done in this chapter for CCI insulators in one dimension; please refer to Refs. [17, 20, 21, 24, 25] for details.

Chapter 3

Physical Consequences of the Topological term in Odd Spatial Dimensions

In this chapter, we will discuss in general how the presence of the topological term (θ term) in odd spatial dimensions changes the physics in a system without boundary, despite being a total derivative. We will start from the effective theory in one and three spatial dimensions, and observe their consequences. We then turn back to one dimension, and check that the effect is sensible in a practical example. This leads to an interesting realization that the Berry's phase from the electrons is actually not gauge invariant. The lattice ions, even if we assume they cannot move, can contribute a non-trivial Berry's phase. Finally, we briefly touch on how non-topological properties, such as the dielectric constant, can affect the result.

3.1 θ-term in one spatial dimension

The θ-term in 1d is defined as

$$\mathcal{L}_{\theta,1D} = \frac{e\theta}{2\pi}\epsilon^{\mu\nu}\partial_\mu A_\nu, \tag{3.1}$$

which is exactly what we have found in the previous chapter, with $\theta = \pi$ describes the CCI topological insulator.

Our strategy consists of two steps: first we show that the θ-term in the path integral is

equivalent to a prescription of forming gauge invariant states. Then we use the Hamiltonian formalism with the free Maxwell Hamiltonian with those states to calculate the partition function at finite temperature. Please see App. A for a derivation directly using the path integral.

Let us first take the $A_0 = 0$ gauge. Define $\tilde{A}_1(q) = \int A_1 \exp(-iqx)\mathrm{d}x$ as the Fourier transform of A_1. On a circle of circumference L, configurations satisfying $\int A_1 \mathrm{dx} \equiv \tilde{\mathrm{A}}_1(0) = 0$ can be gauge transformed into configurations satisfying $\tilde{A}_1(0) = 2\pi n/e$, with n an integer (the winding number). Therefore, when we consider a state that is an eigenstate of the quantized operator $\tilde{A}_1(0)$, say, with eigenvalue 0, we should consider instead a linear combination of all states, each with eigenvalue $2\pi n/e$. The linear combination has to be gauge invariant, and the remaining arbitrary choice would be the phase between states with consecutive n. We call this relative phase θ and call the vacuum of this phase the θ-vacuum:

$$|\theta, \mathrm{phys}\rangle = \sum_n \exp(-i\theta n)|n, \mathrm{phys}\rangle. \tag{3.2}$$

Notice that if we write down the path integral from some state with winding n to some other state with winding m by turning on $A_1(t)$, the winding number can be written as an integral:

$$m - n = \frac{e}{2\pi}\int_n^m \mathrm{dxdt}\frac{\partial \mathrm{A}_1}{\partial \mathrm{t}}; \tag{3.3}$$

here the limits of the integral denote the winding number of the initial and final configuration. The vacuum-vacuum amplitude can thus be expressed as

$$\begin{aligned} & \sum_{m,n}\langle m, 0|\exp(iHt)|n, 0\rangle \exp(i\theta(m-n)) \\ = & \sum_{m,n}\int_{n,0}^{m,0}[DA_1]\exp(iS + i\frac{e\theta}{2\pi}\int \mathrm{dxdt}\frac{\partial \mathrm{A}_1}{\partial \mathrm{t}}); \end{aligned} \tag{3.4}$$

here S in the exponent is just the ordinary action corresponding to H and the scripts of the integral specifies the initial and final boundary conditions. The θ-vacuum description is thus equivalent to adding $\mathcal{L}_\theta$ to the Lagrangian.

Now we proceed to derive the physical consequence of the term. Consider a Maxwell Lagrangian with vacuum angle θ at finite temperature $1/\beta$. Taking $A_0 = 0$, the Maxwell

Hamiltonian is

$$H = \sum_q \frac{1}{2L} \left| \frac{\partial \tilde{A}_1(q)}{\partial t} \right|^2 = \sum_q \frac{1}{2L} |\tilde{E}^1(q)|^2 \equiv \sum_q H_q \tag{3.5}$$

Since $\tilde{A}_1(q \neq 0)$ decouples from $\tilde{A}^1(0)$ we can calculate them independently. θ only couples to the $q = 0$ sector as all operators at finite q have the same eigenvalue for states which differ by arbitrary winding. Let us focus on the partition function of the $q = 0$ sector:

$$Z_{q=0} = \mathrm{Tr}_\theta(e^{-\beta H_0}) = \frac{e}{2\pi} \int_0^{2\pi} \mathrm{d}\phi \int_{-\infty}^{\infty} \frac{\mathrm{d}\ell}{2\pi} \sum_{\mathrm{m}} \sum_{\mathrm{n}} \langle \phi + 2\pi \mathrm{m} | \ell \rangle \langle \ell | \mathrm{e}^{-\frac{\beta \mathrm{L} e^2}{2} \ell^2} | \ell \rangle \langle \ell | \phi + 2\pi \mathrm{n} \rangle \mathrm{e}^{\mathrm{i(m-n)}\theta}; \tag{3.6}$$

the subscript θ denotes that we only trace over the sector whose vacuum is the θ-vacuum. $\phi = e\tilde{A}(q = 0, \tau = 0)$ is the initial configuration of the gauge field. Note that we have inserted $1 = \int_{-\infty}^{\infty} \frac{\mathrm{d}\ell}{2\pi} |\ell\rangle\langle\ell|$, where ℓ is the eigenvalue of $(\tilde{E}^1(q = 0)/eL)$ and $|\ell\rangle$ the eigenstate. The canonical conjugate pairs (x, p) can be determined from the Lagrangian with $p = \frac{\partial \mathcal{L}}{\partial \dot{x}}$; if we choose $(e\tilde{A}^1(q = 0))$ as x it conjugates to $(\tilde{E}^1(q = 0)/eL)$. Therefore we have

$$\langle \phi + 2\pi m | \ell \rangle = \exp(i(\phi + 2\pi m)\ell). \tag{3.7}$$

There is translational symmetry in m and n and the sum over $m + n$ just gives an overall normalization constant. If we replace $(m - n)$ by n, we have

$$Z_{q=0} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\ell}{2\pi} \sum_n e^{in(\theta + 2\pi\ell)} e^{-\frac{\beta L e^2}{2} \ell^2}. \tag{3.8}$$

If we sum over n first, we have

$$\sum_n e^{in(\theta + 2\pi\ell)} \sim \sum_m \delta(\frac{\theta}{2\pi} + \ell + m). \tag{3.9}$$

Physically, this means the effect of the uniform θ term is to cause the average electric field to be quantized in integer units of charges, but shifted by $e\theta/2\pi$. This is a well-known result with open boundary conditions[26], where one can imagine fractional charges at the end produce the electric field. With periodic boundary conditions it is less intuitive.

If $\theta = \pi$, this would imply that the vaccum has two degenerate configurations characterized by $\frac{1}{L} \int \mathrm{dxE} = \pm \frac{1}{2} \mathrm{e}$. The matrix elements between the two states become exponentially small as $L \to \infty$, so we should think of this as a sponteneous symmetry breaking situation

where the parity (P) and charge-conjugation (CC) symmetry are sponteneously broken by the electric field. The electric field would choose one direction and stay for a time period proportional to e^L.

3.2 Physical Consequence of the θ term in Three Spatial Dimensions

Now we turn our attention to three dimensions. In 3d, the topological term is of the form

$$\mathcal{L}_\theta = \frac{\theta e^2}{32\pi^2}\epsilon^{\mu\nu\lambda\omega}\mathrm{tr}(F_{\mu\nu}F_{\lambda\omega}). \tag{3.10}$$

We consider two settings without boundaries: the first is a 3-torus, and the second is the 3-sphere. We restrain ourselves to consider only U(1) gauge fields.

Abelian gauge field on a 3-torus:

Since we need a periodic lattice to produce the topological insulator, it is natural first to consider the world as a 3-torus. Again taking the gauge choice $A_0 = 0$, the θ-term in three spatial dimensions can be written as a difference of the Chern-Simons term on the initial and the final states in the imaginary time direction:

$$\begin{aligned}\int_S \mathrm{d}^4x\mathcal{L}_\theta &\propto \int_S \frac{\mathrm{d}^4x}{8\pi^2}\epsilon^{\mu\nu\lambda\gamma}\partial_\mu A_\nu\partial_\lambda A_\gamma \\ &= \int_{\partial S}\frac{\mathrm{d}^3x}{8\pi^2}A_i\partial_j A_k\epsilon^{ijk},\end{aligned} \tag{3.11}$$

where i, j, k now run through only the spatial directions. One superficial difference to the situation in 1D is that it seems all finite-q components contribute. However, as we require the initial and final states to differ from each other only by a gauge transformation, $\vec{A}_{\text{final}} = \vec{A}_{\text{initial}} + \nabla\phi/e$, we can see the integral on the three-dimensional boundary becomes a total derivative,

$$\int \mathrm{d}^3x\partial_i(\phi\partial_j A_k\epsilon^{ijk}/e) = \int \mathrm{d}^3x\partial_i(\phi B_i). \tag{3.12}$$

Let us assume ϕ only has a winding in the z direction, i.e., $\phi(x, y, L_z) - \phi(x, y, 0) = 2\pi n$, then Eq. (3.12) becomes $2\pi n\Phi_B$ where Φ_B is the total flux threading the torus in the z

direction. Assuming $\Phi_B = m\Phi_0$ with $\Phi_0 = hc/e = 2\pi/e$, we find

$$\int_S \mathrm{d^4x}\epsilon^{\mu\nu\lambda\gamma}\partial_\mu \mathrm{A}_\nu \partial_\lambda \mathrm{A}_\gamma = \frac{8\pi^2}{\mathrm{e}^2}\mathrm{nm}, \tag{3.13}$$

Thus, with m units of the fundamental flux quantum in the z direction, the "θ-vacuum" consists of linear superposition of states with configurations satisfying $\int A_z \mathrm{dz} = 2\pi\mathrm{n/e}$, where n is an integer. Since the Hamiltonian is still quadratic, we can calculate the relevant part of the partition function similar to the calculation in 1D. The analog of Eq. (3.8) is

$$\begin{aligned} Z_{q=0} &\sim \sum_{m,n} \int \frac{\mathrm{d}\ell}{2\pi} e^{imn\theta} e^{i2\pi n\ell} \exp\left(-\frac{\beta V}{2}((\frac{e\ell}{L_x L_y})^2 + (\frac{2\pi m}{eL_x L_y})^2)\right) \\ &\sim \sum_{m,n'} \int \frac{\mathrm{d}\ell}{2\pi} \delta(\frac{m\theta}{2\pi} + \ell + n') \exp\left(-\frac{\beta V}{2}((\frac{e\ell}{L_x L_y})^2 + (\frac{2\pi m}{eL_x L_y})^2)\right). \end{aligned} \tag{3.14}$$

$V = L_x L_y L_z$ is the world volume and we choose our conjugate variables to be $(e\int A_z \mathrm{d^3x/L_x L_y})$ and $(\int E_z \mathrm{d^3x/eL_z})$, with the eigenvalue of the latter labeled by ℓ. We find that with a fix flux $\Phi_B = m\Phi_0$ in the z direction, the electric flux in the same direction is quantized:

$$E_z L_x L_y = e(n - m\theta/2\pi) = ne - \theta\Phi_B/\Phi_0^2, \tag{3.15}$$

with n an integer.

Let us first take the strict $T = 0$ limit. Here the thermal fluctuation of the magnetic flux is suppressed and we find that, the θ-term only has nontrivial effect if there is a finite flux threading through. For $\theta = \pi$, when we have an odd magnetic flux, the electric flux in the same direction would be quantized in half units of e. The electric field goes to zero if the world volume goes to infinity, however.

At finite T, the thermal fluctuation of the magnetic field can generate some finite fluxes, and we would have some effect even with $B = 0$ in average. For simplicity let us again set $\theta = \pi$ and consider $L_x = L_y = L_z = L$. If $T \gg 1/L$, The correlation function of the electric field would contain an extra term comparing to the usual Maxwell theory:

$$\langle E(x)E(y)\rangle \sim \langle E(x)E(y)\rangle|_{\theta=0} + \frac{e^2}{8L^4}. \tag{3.16}$$

One can understand this constant correlation by imagining that half of the states in

the ensemble have an odd number of magnetic fluxes. The state with an odd number of fluxes would have a ground state electric field squared to $(e/2L^2)^2$, and the average is just a half of that. This extra part of the correlation function is long ranged, and can easily be distinguished from the Maxell part. However, the magnitude again vanishes in the large L limit. Since it is not possible to have a 3D torus without embedding it in 4D space, these effects are of academic interests only.

Before we end this subsection, we should note that from this calculation, it is clear that any local magnetic field will not produce any effect. Therefore, one would not see an electric field inside a solenoid, nor any charge at the end of it.

Abelian gauge field on a 3-sphere and magnetic monopoles:

Since we cannot have global nonzero magnetic flux in any direction in a 3-sphere, there will be no effect of the θ-term. This is in contrast to the case with a magnetic monopole, where it is predicted that there will be charge $e(n - \theta/2\pi)$ attached to it in a θ-vacuum. This effect can be understood as follows: magnetic monopole is a singularity in terms of the abelian gauge field. Suppose we have a pair of monopole-antimonopole far away in a 3-sphere so that we have one fundamental flux going from one to the other. The geometry is now a 3-sphere with two punctures. From the calculation of the previous section we can see the electric flux threading from one hole to the other must be quantized, $\Phi_E = e(n - \theta/2\pi)$, and we would attribute this as the charge of the magnetic monopole. Franz et. al. shows that there is Witten effect inside the topological insulator[27]; i.e., a magnetic monopole carries half unit of charge e. This shows up in numerics as a zero energy electronic state localized near the monopole.

As a side note, if we consider nonabelian gauge fields, the θ-term in general does have effect in a 3-sphere. This effect, however, is usually associated with the physics of instantons and is quite different from what we have discussed.

3.3 SSH Model, and the Gauge Invariance of θ

From the discussion of Sec. 3.1 and the discussion in the previous chapter, we realize that in a CCI topological insulator, there will be a ground state electric field $\pm\frac{e}{2}$, if we ignore the screening effect. This observation, however, seems puzzling when one considers the well-known Su-Schreiffer-Heeger (SSH) model[28, 29]. If we consider spinless electrons, the

two ground states in this model will have the effective θ-term with θ which differs by π. The discussion in Sec. 3.1 then suggests that the two ground states have different electric fields. On the other hand, the two states are related by a lattice translation of a (where the doubled unit cell is of period $2a$) and are physically identical. They thus cannot have different electric fields. How do we compromise the two seemingly contradictory statements?

Let us start by reviewing the SSH model. The SSH model is given by the following Hamiltonian in 1D[28]:

$$H = \sum_{i,\sigma}(-t + (-1)^i \Delta) c^\dagger_{i\sigma} c_{i+1\sigma} + h.c., \tag{3.17}$$

Δ takes either positive or negative values for the two ground states which spontaneously break the lattice translation symmetry. Suppose we plug in the wave function

$$\psi_k = a_k \sum_{i \in \text{odd}} c^\dagger_i |0\rangle \exp(ikx_i) + b_k \sum_{j \in \text{even}} c^\dagger_j |0\rangle \exp(ikx_j), \tag{3.18}$$

The Hamiltonian can be put into a matrix form:

$$H_k \begin{pmatrix} a_k \\ b_k \end{pmatrix} = (-2t\cos(ka)\sigma_x + 2\Delta \sin(ka)\sigma_y) \begin{pmatrix} a_k \\ b_k \end{pmatrix}; \tag{3.19}$$

σ_x and σ_y are Pauli matrices and a is the lattice spacing. The Hamiltonian is charge conjugation invariant if we take the charge conjugation operator to be $\sigma_z K$. Notice that H_k is *not* periodic in π/a; nevertheless ψ_k is periodic (up to a phase.) When we apply a small electric field, the coupling enters via Peierls substitution, and directly results in $H_k \to H_{k+eA}$, where A is the spatial part of the gauge field. At half filling where the system is insulating, following our previous discussion, we can calculate the Berry's phase accumulated when we adiabatically turn on the electric field until the system reaches the state related to the initial state by a large gauge transform of winding number one, $A \to A + 2\pi/eL$:[23] (hereafter when we write "the Berry's phase" we refer to the Berry's phase of this procedure)

$$\theta_{\text{Berry}} = \int_{-\pi/2a}^{\pi/2a} i\langle u_k | \frac{\partial}{\partial k} | u_k \rangle \mathrm{d}k, \tag{3.20}$$

with $|u_k\rangle = \begin{pmatrix} a_k \\ b_k \end{pmatrix}$, and we choose the phase convention such that ψ_k periodic in k. If we take $x_n = na$, we can parametrize our solution as

$$|u_k\rangle = \exp\left(\frac{i\mathrm{sgn}(\Delta)f(k)}{2}(\sigma_z - 1)\right)\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{3.21}$$

with

$$\tan(f(k)) = \left|\frac{\Delta}{t}\right|\tan(ka). \tag{3.22}$$

The important thing here is to notice that $f(k) = 0$ at $k = 0$ and $f(k) = \pm\pi/2$ at $k = \pm\pi/2a$. We therefore get

$$\theta_{\text{Berry}} = \mathrm{sgn}(\Delta)\frac{\pi}{2}, \tag{3.23}$$

for each spin.

If we consider the spinful case as in the original SSH model, the total Berry's phase is $2\theta_{\text{Berry}}$, which differs 2π from each other for the two ground states, implying that both would have the same properties. However, since $\theta = \pi$ for both states, we would naively predict that there is a electric field $E \sim \pm e/2$ in both states. This prediction seems rather unlikely. For the spinless case, the situation is even worse, as the θ differs by π between the two states, generating a different static electric field. Yet, the two states are related by a lattice translation of a, and should be physically equivalent.

These paradoxical observations can be resolved, if we realize that the charged ions can also have a Berry's phase. It is somewhat surprising in the sense that the ions are considered to be stationary localized charges and behave rather trivially. To see how the Berry's phase comes about, we have to recall how the Berry's phase is properly defined. In order to define the Berry's phase when the state adiabatically transforms into another state which is related to the original state by a large gauge transform, we first have to identify the two states as two different descriptions of the same physical state.[30] Therefore they have to correspond to the same physical state up to a definite phase. Consider a Bloch wave function $\psi_k(x) = u_k(x)\exp(ikx)$, under the large gauge transform of winding number one, it becomes

$$\psi_k(x) \to \bar{\psi}_k(x) \;\; = \;\; \psi(x)\exp(-i2\pi x/L)$$

$$= u_k(x)\exp(i(k-2\pi/L)x); \tag{3.24}$$

L is the size of the lattice. Without loss of generality, let us identify the two wave functions (that is, to assume the two wave function describe the same physical state with identical phases):

$$u_k(x)\exp(ikx) \sim u_k(x)\exp(i(k-2\pi/L)x). \tag{3.25}$$

For consistency, this identification should stay the same for any $u_k(x)$.

Now let us shift both wave functions by x_0:

$$\begin{aligned}
\psi'_k(x) &= u_k(x-x_0)\exp(ik(x-x_0)) \\
&= (u_k(x-x_0)\exp(-ikx_0))\exp(ikx) \\
&\equiv u'_k(x)\exp(ikx). \qquad (3.26) \\
\bar{\psi}'_k(x) &= u_k(x-x_0)\exp(i(k-2\pi/L)(x-x_0)) \\
&= u'_k(x)\exp(i(k-2\pi/L)x)\exp(i2\pi x_0/L) \qquad (3.27)
\end{aligned}$$

We can regard $u'_k(x)$ as the periodic part of some other wave function. Therefore, with the identification Eq. (3.25), we must have

$$\psi'_k(x) \sim u'_k(x)\exp(i(k-2\pi/L)x) = \bar{\psi}'_k(x)e^{-i2\pi x_0/L}; \tag{3.28}$$

that is, following the same identification, the translated wave function is identified with the translated gauge transform with an additional phase $\phi = (-2\pi x_0/L)$!

This phase shows up in the calculation of the Berry's phase. We have

$$\begin{aligned}
\theta'_{\text{Berry}} &= \int_{-\pi/a}^{\pi/a} i\langle u'_k|\frac{\partial}{\partial k}|u'_k\rangle \mathrm{d}k \\
&= \theta_{\text{Berry}} + 2\pi\left(\frac{x_0}{a}\right). \qquad (3.29)
\end{aligned}$$

The extra Berry's phase is compensated by the extra phase in Eq. (3.28), after summing over (L/a) states in the Brillouin zone.

This "non-invariance" of the identification under translation" arises from the fact that the gauge transform does not commute with translation. The discussion above shows that this Berry's phase for a single charged wave function is not a physical quantity. It depends

on how one identifies the wave functions related by a large gauge transform; however, for a given identification, the wave functions are identified differently when they are translated.

Nevertheless, the total phase difference in the identification for a product of single particle wave functions when the state are translated by x_0 equals $N\phi$, where N is the total charge. For a charge-neutral system, the total Berry's phase is therefore invariant under the translation of the whole system. Since the translation changes the position of the ions, the Berry's phase, or the coefficient of the θ-term, is not determined only by the "topology" of the occupied bands, but also reflects their relative position to the ionic lattice. A translation of only the electrons or only the ions will result in a different Berry's phase, and a different ground state electric field.

Let us now return back to the original problem. In the spinless case, the ions should have the same density as the electrons, which is half a charge per unit cell. If the ions are localized, they would have a $2a$ period. For the two degenerate ground state, the ionic states are related by a shifted of a. Now that we know that a half-period shift of the ions will also give a Berry's phase differed by π, the total Berry's phase is indeed the same for the two ground states.

One might wonder how this argument applies for a jellium-like ionic state. The translated ions can look very similar to the original state, and it seems paradoxical for them to have such different Berry's phases. Here we argue that, despite the similarity in the density profile, since we only have one ion per two lattice spacing, the translated state is always very different from the original state, as long as the ions are localized. This is most evident when we look from the single-particle perspective. The center-of-mass positions of the ions must differ by $2a$, and the product wave function is different if we shift it by a. On the other hand, if one thinks about the opposite (unphysical) limit, where the ions are completely delocalized and are described by plane waves, to get rid of any $2a$ periodicity, the ionic state then becomes gapless, and the Berry's phase procedure does not apply. We thus conclude that for an inert ionic lattice with one ion per two lattice spacing, it can only be $2a$-periodic, and a translation of a gives a different state, with a Berry's phase differed by π.

When we derive Eq. (3.23), it is as if we implicitly assume the ions are setting right at $x_n = 2na$ (so that they do not contribute to the Berry's phase.) If we place the ions at the places where most electrons are, $x_n = \mathrm{sgn}(\Delta)\frac{1}{2}a + 2na$, the total Berry's phase for both

ground states are zero. Fig. (3-1) summarizes the result.

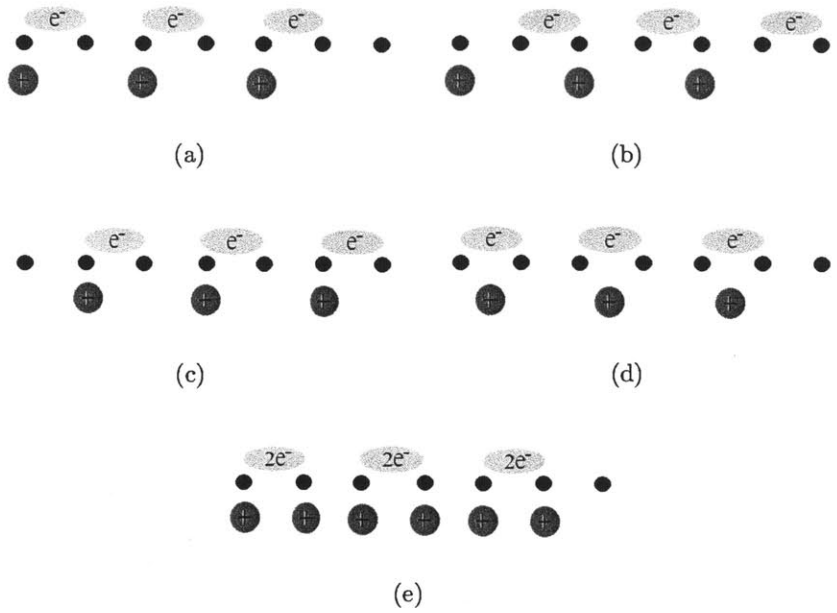


Figure 3-1: (a)-(d) refers to the spinless case. (a) One of the electronic "ground state", without considering the ions. It is predicted in this state there is a -e/4 static electric field. (b) The other "ground state", without changing the lattice. Evidently the two state are different. (c) The other ground state with ions shifted. Now the physics is identical to (a). Even though we draw point-like ions here, the argument actually works for any charge distribution, including jellium as a limiting case. (d) If the ions are at the lowest energy positions, the ground state electric field is zero. (e) For the spinful case, a simple consideration would show that this configuration will have zero ground state electric field.

For the spinful case, since the number of ions are doubled, the difference between the Berry's phases of the two states is also doubled. The lattice contribution for the two states therefore differs by 2π, which implies that shifting the lattice by a does not change the ground state property, as expected. To get the correct expression for θ however, we still have to consider the ionic contribution to the Berry's phase. The π Berry's phase we obtained eariler does not include the ionic contribution, which is equivalent to assuming they are placed at $x_n = 2na$, with two ions at the same site. If we shift half of the ions by a, forming the usual lattice with period a, the total Berry's phase will again be shifted by π, and there will be no ground state electric field.

Closing this section, we note that if we view θ as the polarization[23, 31], it seems almost trivial to say that it must depend on the ionic lattice. Nevertheless, the famous

formula for polarization, Eq. (2.17) Our argument thus provides a simple picture which complements the conventional view of polarization with open boundaries conditions. It is especially helpful with unit cell doubling, as in the conventional view, the termination of the crystal with doubled unit cell complicates the problem.

3.4 Effect of the Dielectric Constant

In a one dimensional world, a electric field with magnitude $e/2$ is huge. In a topological insulator with $\theta = \pi$, it is thus natural to ask whether the generated electric field can somehow be screened to lower the total energy. In addition, if the electric field is not screened, it then becomes an universal signature of the 1D topological insulator. With open boundary conditions, the static electric field is screened by the dielectric constant. This screening corresponds to a net displacement between the electrons and the ions, which accumulates charge at the two ends and creates an electric field in the reverse direction. With periodic boundary conditions, no charges are accumulated from such displacement; however, from the discussion in the previous section, we now know this displacement changes the θ. We therefore are set to answer the question, whether the screening with periodic boundary conditions is the same as with open boundary conditions.

We first start from an effective theory with a built-in dielectric constant:

$$\mathcal{L}_{1D} = -\frac{\epsilon}{4}(F_{\mu\nu})^2 + \frac{e\theta}{2\pi}\epsilon^{\mu\nu}\partial_\mu A_\nu = \frac{\epsilon}{2}E^2 + \frac{e\theta}{2\pi}E. \tag{3.30}$$

Let us again write down the $q = 0$ sector of the partition function:

$$Z_{q=0} \propto \int_0^{2\pi} \mathrm{d}\phi \int_{-\infty}^{\infty} \frac{\mathrm{d}\ell}{2\pi} \sum_{\mathrm{m,n}} \langle \phi + 2\pi\mathrm{m}|\ell\rangle\langle\ell| \exp(-\frac{\beta \mathrm{L} \mathrm{e}^2}{2\epsilon}\ell^2)|\ell\rangle\langle\ell|\phi + 2\pi\mathrm{n}\rangle \mathrm{e}^{\mathrm{i}(\mathrm{m}-\mathrm{n})\theta}; \tag{3.31}$$

again, ϕ is the initial value of $(e\tilde{A}^1(q = 0))$. Note that we now choose ℓ to be the eigenvalue of the operator $(\epsilon\tilde{E}^1(q = 0)/eL)$, hence the factor of ϵ in the denominator of the exponent. Notice that with the modified Lagrangian, it is now $(\epsilon\tilde{E}^1(q = 0)/eL)$ which is conjugate to $(e\tilde{A}^1(q = 0))$. Therefore,

$$\langle \phi + 2\pi m|\ell\rangle = \exp(i(\phi + 2\pi m)\ell) \tag{3.32}$$

remain unchanged.

Now we can follow through the same calculation, realizing that *it is ℓ that is quantized.* The ground state electric field, following the same argument, should instead be

$$E = -\frac{\theta e}{2\pi\epsilon}, \ -\pi < \theta < \pi. \tag{3.33}$$

This matches the situation with open ends. The ground state electric field is thus screened as well with periodic boundary conditions and does not take an universal value.

On the other hand, one should also be able to start from vacuum, and understand the screening as a dynamical effect. In the last section, we have found that θ shifts by 2π as we shift the electronic wave function by a lattice period. It is thus intuitive to think, that the electrons will shift a little bit, responding to the electric field generated from the θ-term, and make θ smaller. Here we are going to show that this intuitive picture gives precisely the same effect as above.

From the point of view of the charges, θ is the Berry's phase when the system slowly transit from its ground state to another state which is related by a large gauge transform. In the adiabatic limit, we derive that the phase is just the topological index. However, since the θ-term in turn predicts that there in a finite electric field in the ground state, the procedure is actually far from the adiabatic limit, and there can be some extra dynamical phases.

Instead of calculating the dynamical phases in detail, let us switch and suppose we already have the effective theory, with some parameter θ and ϵ. From the effective theory point of view, the accumulated phase in the presence of a finite field is just the first derivative of the electronic action with respect to the electric field. This gives

$$\theta_{\text{Berry}} = \theta + \frac{2\pi}{e}(\epsilon - 1)E. \tag{3.34}$$

We then proceed with the quantization of the gauge field in vacuum with this modified θ_{Berry}. We get

$$E = -\frac{\theta_{\text{Berry}} e}{2\pi} = -\frac{\theta e}{2\pi} - (\epsilon - 1)E, \tag{3.35}$$

and we recover the same result as Eq. (3.33). This calculation matches our intuition that the wave function can adjust itself a little bit (a compromise between a rigid shift and the

ionic potential, characterized by the dielectric constant ϵ) to reduce the electric field.

We have to note that the second treatment does not work at finite temperature, as witnessed by the different quantization of the electric field in the two methods. At finite temperature, the electric field fluctuates from the average value. Once the electric field fluctuates around, it would be wrong to identify the contribution from the dielectric constant as a phase, instead of an energy. Nevertheless, one can still expect that treating it as a phase should give correct ground state properties at zero temperature. Physically this is because in the ground state the partition function is dominated by the states with the average electric field. When one calculates the phase accumulated when the gauge winding increases with a fixed electric field, there is no real distinction between the contribution from the geometric Berry's phase and the dynamical phase.

Chapter 4

Topological Responses from Conventional Perturbation Theory

Stepping toward higher spatial dimensions, we expect to observe topological responses at higher orders of the external fields, as we see in Sec. 1.3.2. While we have derived the θ term in one spatial dimensions calculating a Berry's phase, traditionally the effective action is obtained by integrating out the fermionic bands in momentum space. The integration is carried out in momentum space, and the effective action is generated by the one-loop diagrams with external fields as external legs.

In this chapter we shall investigate the limitation of deriving topological responses from the conventional approach. We will describe a (not so successful) method trying to isolate contributions from the topological index of the bands. We shall see that in principle this method can capture topological responses in even spatial dimensions, but has to rely on edge or pumping responses to capture the topological responses in odd spatial dimensions.

4.1 Perturbation Theory in Energy Eigenbasis

Starting from a general translation-invariant tight-binding Hamiltonian, we have

$$H = \sum_{<i,i+\vec{d}>,\vec{d}} c^{\dagger}_{i,m} c_{i+\vec{d},n} t^{\vec{d}}_{mn} \exp(iA_{i,i+\vec{d}}) \tag{4.1}$$

where i, j are site indices, m, n are internal, i.e., orbital and spin indices, and $\vec{d}$ runs through all neighboring hoppings. $A_{i,i+\vec{d}} = \vec{A}(\vec{x}_i + \vec{d}/2) \cdot \vec{d}$ is the lattice gauge field derived from the external electromagnetic field. Fourier transforming, we get in the momentum space (suppressing internal indices from here on)

$$H = \sum_{k,q,d} c^\dagger_{k+q/2} h^{\vec{d}}_k c_{k-q/2} \sum_x \exp(i\vec{A}(x) \cdot \vec{d} + i\vec{q} \cdot \vec{x}) \tag{4.2}$$

where $h^d_k = t^{\vec{d}} \exp(i\vec{k} \cdot \vec{d})$. Now if we expand in powers of $\vec{A}$ and sum over $\vec{d}$, we get

$$\begin{aligned} H &= \sum_k c^\dagger_k h(k) c_k + \sum_{k,q} c^\dagger_{k+q/2} \vec{A}(-q) \cdot \frac{\partial h(k)}{\partial \vec{k}} c_{k-q/2} \\ &\quad + O(\vec{A}^2), \end{aligned} \tag{4.3}$$

again where $h(k) = \sum_d h^{\vec{d}}_k$. All the information about the system is encoded in the mapping from the Broullin zone (BZ) to $h(k)$. Now we go to the basis which diagonalizes $h(k)$ and also expand in power of q (suppressing dependence on k if appropriate):

$$\begin{aligned} H &= \sum_k d^\dagger_k \mathcal{E}(k) d_k + O(\vec{A}^2) \\ &\quad + \sum_{k,q} d^\dagger_{k+q/2} \vec{A}(-q) \cdot \left(\frac{\partial \mathcal{E}}{\partial \vec{k}} + [\vec{\Lambda}, \mathcal{E}] + O(q^2) \right) d_{k-q/2} \\ &\quad - \frac{1}{2} \sum_{k,q} d^\dagger_{k+q/2} \{ \vec{A}(-q) \cdot \frac{\partial \mathcal{E}}{\partial \vec{k}}, \vec{q} \cdot \vec{\Lambda} \} d_{k-q/2} \\ &\quad - \frac{1}{2} \sum_{k,q} d^\dagger_{k+q/2} \{ \vec{A}(-q) \cdot [\vec{\Lambda}, \mathcal{E}], \vec{q} \cdot \vec{\Lambda} \} d_{k-q/2}. \end{aligned} \tag{4.4}$$

In this equation, $\mathcal{E}(k)$ is a diagonal matrix of energies with momentum k so that $h(k) = \mathcal{U}(k)\mathcal{E}(k)\mathcal{U}^\dagger(k)$; $d_{k,m} = \sum_n \mathcal{U}^\dagger_{mn}(k) c_{k,n}$ is the energy eigenstate, and $\vec{\Lambda}(k) \equiv \mathcal{U}^\dagger(k)(\partial_{\vec{k}} \mathcal{U}(k))$. $[..., ...]$ and $\{..., ...\}$ are commutators and anticommutators, respectively.

The information of the system now splits into ϵ and U. An insulator means that there is a finite energy gap at every k, between occupied and unoccupied states. At a specific momentum k, small deformations of the Hamiltonian can change the energy or mix occupied and empty states within themselves without closing the gap. The topological information of the band structure, therefore, is stored in U, with an identification with arbitrary unitary transformations within occupied/empty states acted upon. The possible topological

classification is then derived from a mapping from a d-dimensional torus (the BZ) to the space $\frac{U(n+m)}{U(n)\times U(m)}$. Specifically, in even spatial dimensions, the Chern number is one of the topological indices that can be written as an integral that depends only on U.

To write the Chern numbers in terms of $\vec{\Lambda}$, let us relate it to the usual Berry's gauge field defined in the BZ:

$$\begin{aligned}
\mathcal{A}^i_{\alpha\beta} &\equiv -i\langle\alpha|\frac{\partial}{\partial k_i}|\beta\rangle = i\langle 0|d_\alpha(\frac{\partial}{\partial k_i}d^\dagger_\beta)|0\rangle \\
&= -i\langle 0|c_n U^\dagger_{\alpha n}(\frac{\partial}{\partial k_i}U_{m\beta})c^\dagger_m|0\rangle \\
&= -i\Lambda^i_{\alpha\beta}, \qquad (4.5)
\end{aligned}$$

where $|0\rangle$ denotes the empty vacuum; α and β run through occupied bands. We can readily evaluate the field strength:

$$\begin{aligned}
\mathcal{F}^{ij}_{\alpha\beta} &= \partial_i a^j_{\alpha\beta} - \partial_j a^i_{\alpha\beta} + i([a^i, a^j])_{\alpha\beta} \\
&= -i\sum_{\gamma\in\text{occ}}(\Lambda^i_{\alpha\gamma}\Lambda^j_{\gamma\beta} - (i\leftrightarrow j)). \qquad (4.6)
\end{aligned}$$

All the Chern classes can be written as integral involving $\vec{\mathcal{A}}$ and $\vec{\mathcal{F}}$, thus can be expressed using $\vec{\Lambda}$. For example the first Chern number is just $\int \mathrm{d}^2k\epsilon^{ij}\mathrm{tr}(\mathcal{F}_{ij})$ and the second Chern number is $\int \mathrm{d}^4k\epsilon^{ijk\ell}\mathrm{tr}(\mathcal{F}_{ij}\mathcal{F}_{k\ell})$.

Now that we have some topological index in mind, we can use Eq. (4.4) to derive the effective action of the electromagnetic field and look for the right combination. For the response to be topological we expect exact cancellation of ϵ from the propagators and the vertices. We can also count the power of $\vec{\Lambda}$ in a diagram toward the expression of the index.

Before we dig into the calculation, note that the electromagnetic field is not the only possible external field. We should add interactions as we see fit and calculate the effective action in the enlarged sector. Here we introduce two additional terms:

$$\begin{aligned}
H_V &= \sum_{k,q} c^\dagger_{k+q/2}V(-q)c_{k-q/2} \\
&= \sum_{k,q} d^\dagger_{k+q/2}(1-\vec{q}\cdot\vec{\Lambda}+O(q^2))V(-q)d_{k-q/2}, \qquad (4.7) \\
H_\Delta &= \sum_{k,q} d^\dagger_{k+q/2}([\mathcal{E},\Delta]f(-q)+O(q^2))d_{k-q/2}
\end{aligned}$$

$$-\frac{1}{2}\sum_{k,q} d^{\dagger}_{k+q/2}\{[\mathcal{E},\Delta],\vec{q}\cdot\vec{\Lambda}\}f(-q)d_{k-q/2}. \tag{4.8}$$

H_V is just the coupling to the electric potential. H_δ, on the other hand, requires some explanation. In addition to bulk effective actions we would also like to address implications on the boundary. In some cases we can model the boundary as a gradual change in the Hamiltonian. Imagine a term

$$\delta H = \sum_{ij} c^{\dagger}_i f(\frac{\vec{x}_i+\vec{x}_j}{2})\delta h_{ij} c_j, \tag{4.9}$$

where f is an envelop function, interpolating between 0 and 1; h_{ij} is translationally invariant and only depends on the difference between i and j. Now Fourier transform it, we have

$$\delta H = \sum_{k,q} c^{\dagger}_{k+q/2}\delta h(k) f(-q) c_{k-q/2}. \tag{4.10}$$

Finally, since non-topological edge properties are not generic, we may as well assume that the energies are not modified and take δh_k to be of the form

$$\delta h(k) = \mathcal{U}^{\dagger}(1+\Delta^{\dagger})\mathcal{E}(1+\Delta)\mathcal{U} - \mathcal{U}^{\dagger}\mathcal{E}\mathcal{U} \simeq \mathcal{U}^{\dagger}[\mathcal{E},\Delta]\mathcal{U} \tag{4.11}$$

with $\delta^{\dagger} = -\delta$, which describes a k-dependent small rotation of the energy eigenbasis. Writing it using the eigenbasis we would arrive at Eq. (4.8).

One might wonder that the contributions from order of $\vec{A}^2$, q^2, or higher cannot be ignored, especially in higher order diagrams. This is in fact the case, but we can partly escape from dealing with those if we (i) use as many V as possible via gauge transformations; (ii) antisymmetrize $\vec{A}$'s so that the contributions from the paramagnetic current cancel; and (iii) antisymmetrize the external momentum so that other $O(q^2)$ terms do not contribute. One may realize that these conditions are most easily met when one aims to calculate topological effective actions; and it seems that this is one of the technical reasons why the topological indices of the band structure only appears as coefficients of the topological effective action.

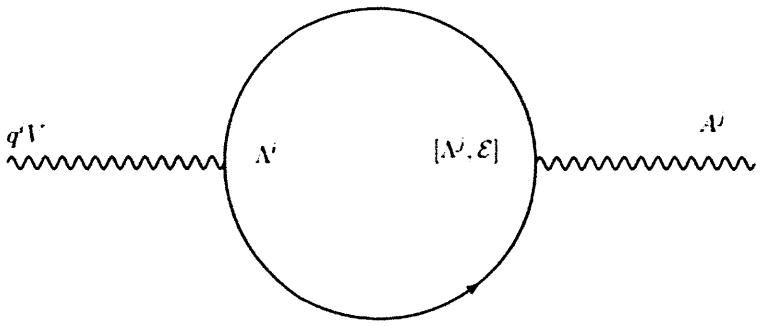


Figure 4-1: The Feynman diagram describing the transverse conductivity.

4.2 Application to One and Two Spatial Dimensions

We start with the integer quantum Hall effect (IQHE). Consider the diagram depicted in Fig. 4-1 which describes a linear response. Based on the formalism above, we will choose one external leg couple to V and the other one to $\vec{A}$. The integral of ω

$$\int \frac{\mathrm{d}\omega}{2\pi} \frac{-1}{i\omega - \epsilon_\alpha} \frac{1}{i\omega - \epsilon_\beta} = \frac{1}{|\epsilon_\alpha - \epsilon_\beta|}, \text{ if } (\epsilon_\alpha \epsilon_\beta) < 0 \tag{4.12}$$

ensures that off-diagonal matrix elements in the vertices are required. Therefore, we have to take the q^1 term in the V vertex, and the $\partial\epsilon$ in the q^0 term with $\vec{A}$ does not contribute. we can immediately see that in the remaining ϵ cancels, and gives

$$\begin{aligned} S_{\text{eff}} \supset & \int \frac{\mathrm{d}^2 q \mathrm{d}\omega}{(2\pi)^3} q^i V(-q) A^j \sum_{\alpha \in \text{occ}, \beta \in \text{emp}} \\ & \left(\int \frac{\mathrm{d}^2 k}{(2\pi)^2} (\Lambda^i_{\alpha\beta} \Lambda^j_{\beta\alpha} - (i \leftrightarrow j)) \right) \qquad (4.13) \\ = & \int \mathrm{d}^2 x \mathrm{d}t \frac{-C_1}{2\pi} (\partial_x V A_y - \partial_y V A_x), \qquad (4.14) \end{aligned}$$

which is the quantized transverse response (in the units $e = \hbar = 1$.) $C_1 \equiv \frac{1}{2\pi} \int \mathrm{d}^2 k \mathrm{Tr}(\epsilon_{ij} f^{ij})$ is the first Chern number. From the gauge invariance we can deduce that the full low energy effective action is of the form

$$S_{\text{eff}} = \int \mathrm{d}^2 x \mathrm{d}t (\frac{C_1}{4\pi}) \epsilon_{ijk} \partial_i A_j A_k \tag{4.15}$$

with $V \equiv A_0$ and i, j, k runs from 0 to 2. Compared with the derivation in Sec. 1.2.3, this method is cleaner and shows cleary how the response does not depend on energetics. On the other hand, we should take note that, despite that in this calculation the total-antisymmetrization tensor naturally appears, it is more due to the gauge invariance than some structure of the Feynman diagram. We will see later in higher order diagrams this automatic anti-symmetrization would not occur.

We should emphasize here that this is a bulk effect, in the sense that the effect exists even in the absence of edges. Experimentally one can verify this doing AC conductivity measurements at a frequency $\omega \ll \Delta$, where Δ is the minimum gap.

Now let us turn our attention to one dimension lower. We know that the polarization can be expressed using the Berry's gauge field:

$$P_x = \int \frac{\mathrm{d}k_x}{2\pi} \mathcal{A}_x. \tag{4.16}$$

The Polarization P_x is only defined modulo one. If we have charge-conjugation symmetry, then P_x can only take the value either 0 or $\frac{1}{2}$. We have shown in Chap. 2 that this distinguishes the two classes of CCI insulators. Hamiltonians with $P_x = 0$ and $P_x = \frac{1}{2}$ cannot smoothly deform into each other preserving charge conjugation.

As we have also shown in Sec. 2.4, the polarization comes in the topological term in the effective action as $(-P \cdot E)$. We can try and see if we recover the same result. Anticipating, we calculate all possible Feynman diagrams which are proportional to Λ_x.

However, all tadpole diagrams vanish identically either by the structure of the vertex or by the momentum conservation which sets $q = 0$. The bubble diagrams are non-vanishing only if there are two factors of Λ_x. It seems we cannot derive such term!

Let us for now look at boundary effects instead. Using H_δ defined above, we can calculate bubble diagrams with one H_δ vertex and one coupling to the gauge field as in Fig. 4-2. If we take the V vertex it gives

$$\begin{aligned} S_{\text{eff}} \supset & \int \frac{\mathrm{d}q\mathrm{d}\omega}{(2\pi)^2} qV(-q)f(q) \sum_{\alpha\in\text{occ},\beta\in\text{emp}} \\ & \left(\int \frac{\mathrm{d}k}{(2\pi)} (\Delta_{\alpha\beta}\Lambda_{\beta\alpha} - \Lambda_{\alpha\beta}\Delta_{\beta\alpha}) \right) \qquad (4.17) \\ = & \int \mathrm{d}x\mathrm{d}t \; V\partial_x f \left(\int \frac{\mathrm{d}k}{(2\pi)} i\mathrm{Tr}_{\text{occ}}([\Delta, \Lambda]) \right). \qquad (4.18) \end{aligned}$$

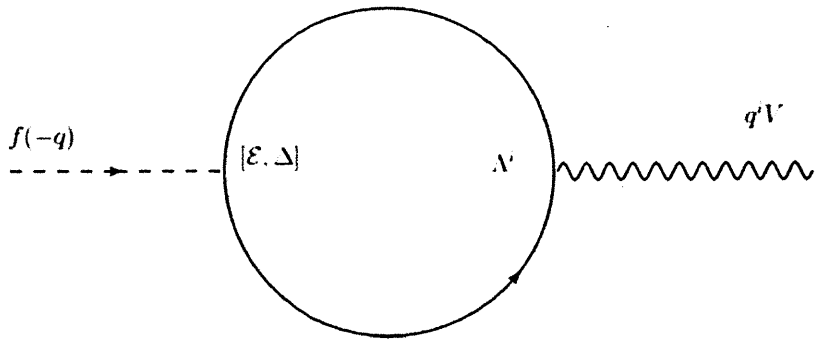


Figure 4-2: The Feynman diagram describing the 1d edge response.

With the A_x vertex the answer would be

$$S_{\text{eff}} \supset \int \mathrm{d}x\mathrm{d}t\ A_x \partial_t f \left(\int \frac{\mathrm{d}k}{(2\pi)} (-i) \mathrm{Tr}_{\text{occ}}([\Delta, \Lambda]) \right). \tag{4.19}$$

Since Δ maps $\mathcal{U} \to \mathcal{U}' = \mathcal{U}(1+\Delta)$, we can say that $\vec{\Lambda}$ is also mapped to

$$\begin{aligned} \Lambda^i \to \Lambda^{i'} &= (1+\Delta^\dagger)\mathcal{U}^\dagger \frac{\partial}{\partial k^i}(\mathcal{U}(1+\Delta)) \\ &= \Lambda^i + [\Lambda^i, \Delta] + \frac{\partial \Delta}{\partial k^i}. \end{aligned} \tag{4.20}$$

Therefore,

$$\int \frac{\mathrm{d}k}{(2\pi)} \mathrm{Tr}_{\text{occ}}([\Delta, \Lambda]) = \int \frac{\mathrm{d}k}{(2\pi)} \mathrm{Tr}_{\text{occ}}(-\delta\Lambda) = -i(\delta P). \tag{4.21}$$

Plugging in, we finally have

$$S_{\text{eff}} \supset \int \mathrm{d}x\mathrm{d}t\ \left(V \partial_x (\delta P) - A_x \partial_t (\delta P) \right). \tag{4.22}$$

Notice that the effective action is now non-vanishing, as we vary the Hamiltonian either in space or in time. Specifically, when P varies spatially there would be a charge $Q \sim \partial_x P$ and when it varies in time, there would be a current $J \sim -\partial_t P$; which is just why this entity is the polarization. Therefore, if one put a CCI 1d insulator with $P = 0$ together with another with $P = \frac{1}{2}$, there would be half a charge localized around the boundary, its sign (and up to multiple integer units of charges) depends on the detail how one smoothly interpolate between the two states. If the charge conjugation symmetry is preserved throughout, then

in the middle there must be a zero mode, as a limit of the two different interpolation whose charges differ by one. When the zero mode is occupied the total charge on the boundary is $+\frac{1}{2}$ and $-\frac{1}{2}$ if it is empty.

One might notice that there is actually an ambiguity in the derivation above. When we Fourier transform back into real space, it seems there is no reason why we should not put the derivative on the external field instead of δ. Indeed, in the current formulation these two choices are equivalent. A total derivative Fourier transforms to zero. Therefore, in this formulation, one needs to vary the Hamiltonian as above to really observe the term.

On the other hand, naively one might expect the absence of a total derivative is a side effect from calculating in the momentum space. This is not the case, however, if we calculate the effective action in 1d, we will get at linear order in A_x

$$\begin{aligned} S_{eff} &\supset \int \mathrm{d}x\mathrm{d}t \sum_{<i,i+\vec{d}>,\vec{d}} \langle c^{\dagger}_{i,m} c_{i+\vec{d},n} \rangle_0 t^{\vec{d}}_{mn} i A_{i,i+\vec{d}} \\ &= \int \mathrm{d}x\mathrm{d}t \ -\langle J_x \rangle_0 A_x \\ &= 0. \end{aligned} \tag{4.23}$$

$\langle ... \rangle_0$ denotes the ground state average, which is just zero. The problem therefore is not that the Fourier transform kills the term, but that the Berry's phase as one adiabatically turns on the electric field is somehow invisible to the conventional perturbation theory.

4.3 Application to Higher Dimensions

This method is not constrained to work only on the bubble diagrams. Nevertheless, as we will see below, working on higher order diagrams such as the triangular diagrams would in general give nonzero results. One must, therefore, focus on the channel interested instead of derive everything at the same order.

As an illustration let us consider the nonlinear electromagnetic response in four spatial dimensions as in Ref. [16, 32]. Let us start, however, by first considering the topological index we are after. The second Chern number is of order Λ^4. If we exclude the V vertex, we have to have either 4 vertices of $\vec{A}$ at q^0 order or 3 vertices with one of them at q^1 order. in both cases we need to calculate at ω^1 order in order to cancel the energy dependence. However, the anti-symmetrization of the subscripts would kill the first term, and the only

possible combination to get the topological index is indeed the triangular diagram which characterizes the nonlinear electromagnetic response. The diagram is depicted in Fig. 4-3. The contribution from this diagram would not be anti-symmetric in q and $\vec{A}$. Indeed, the

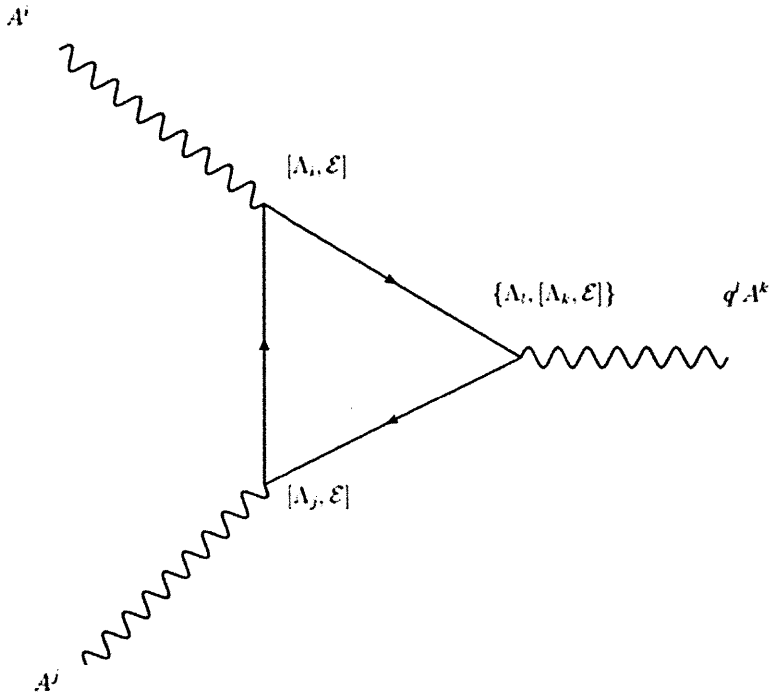


Figure 4-3: The Feynman diagram for the nonlinear transverse conductivity in 4d

effective action contains other nonlinear response terms in addition to the second Chern-Simons term. Nevertheless, we can project onto the anti-symmetrized subspace by the identity

$$\begin{aligned} X_{ijkl}Y^{ijkl} &= \frac{1}{4!}(X_{ijkl}\epsilon^{ijkl})(Y^{i'j'k'l'}\epsilon_{i'j'k'l'}) \\ &\quad +(\text{remaining parts}). \end{aligned} \tag{4.24}$$

Now we simply calculate the diagram, anti-symmetrizing all the indices on $\vec{\Lambda}$. Here we focus on the case where all occupied/unoccupied states are degenerate. We get

$$\begin{aligned} S_{\text{eff}} \supset\ & \frac{S_{4D}}{24}\int \frac{\mathrm{d}\omega}{(2\pi)}\frac{\mathrm{d}^4k}{(2\pi)^4} \sum_{\alpha,\alpha'\in\text{occ},\beta,\beta'\in\text{emp}} \frac{1}{i\omega-\epsilon_\alpha}\frac{1}{i(\omega+\omega_1)-\epsilon_\beta}\frac{1}{i(\omega-\omega_2)-\epsilon_\beta}(\epsilon_\alpha-\epsilon_\beta)^3 \times \\ & P_\alpha\Lambda^\mu P_\beta\Lambda^\lambda P_{\alpha'}\Lambda^\omega P_{\beta'}\Lambda^\nu\epsilon_{\mu\lambda\omega\nu} + (\alpha\leftrightarrow\beta,\ \alpha'\leftrightarrow\beta') \end{aligned} \tag{4.25}$$

where

$$S_{4D} = \int \frac{\mathrm{d}^3 q_1 \mathrm{d}^3 q_2}{(2\pi)^6} \frac{\mathrm{d}\omega_1 \mathrm{d}\omega_2}{(2\pi)^2} \epsilon_{\mu\lambda\omega\nu} (-q_1 - q_2)^\lambda A_1^\mu A_{(-1-2)}^\omega A_2^\nu \tag{4.26}$$

with A_1^μ shorthanded for $A^\mu(-q_1, -\omega_1)$, $P_\alpha \equiv |\alpha\rangle\langle\alpha|$ and vice versa. Taylor expanding to first order in ω_1 and ω_2, integrating out ω, and we would arrive at

$$S_{\text{eff}} \supset \frac{-S_{4D}}{48}(\omega_1 - \omega_2) \int \frac{\mathrm{d}^4 k}{(2\pi)^4} \mathrm{Tr}(f_{\mu\lambda} f_{\omega\nu} \epsilon^{\mu\lambda\omega\nu}). \tag{4.27}$$

Fourier transforming, we obtain the nonlinear electromagnetic response

$$S_{\text{eff}} = \frac{C_2}{12\pi^2} \int \mathrm{d}^4 x \mathrm{d}t \epsilon_{\mu\lambda\omega\nu} \partial_t A^\mu \partial_\lambda A^\omega A^\nu \tag{4.28}$$

with

$$C_2 = \frac{\pi^2}{2} \int \frac{\mathrm{d}^4 k}{(2\pi)^4} \mathrm{Tr}(f_{\mu\lambda} f_{\omega\nu} \epsilon^{\mu\lambda\omega\nu}). \tag{4.29}$$

Several comments are in order. While we didn't show that the result is independent of the dispersion, once one sets to calculate the diagram with flat bands the calculation becomes very simple. In fact, one might argue without calculation that in the anti-symmetrized channel the response must be proportional to the second Chern number, since it is the only "gauge invariant" combination of $\vec{\Lambda}$ with their indices anti-symmetrized; the "gauge invariance" here refers to the emergent extra degrees of freedom when the bands are degenerate so that one can choose the eigenbasis arbitrarily. Since the physical result after integrating out the fermions should be independent of the basis, the response function must endow this gauge symmetry. On the other hand, this term is by no means the only term non-vanishing at the same order. The other terms, however, are not invariant subject to deformation of the bands and are not topological.

From a technical point of view, one might wonder why we did not calculate the response with one vertex being V as before. The reason is that with the anti-symmetrization V is no longer needed to kill the paramagnetic current terms. (In fact one cannot kill the paramagnetic term by using V since there are three A's in the diagram.) In addition, the diagram involving V would contribute at q^2 order instead of $q^1\omega^1$, which proves to be a little bit more troublesome, due to the fact that our q-expansion of the Hamiltonian expands around k, the circling fermion momentum. In triangular or higher order diagrams there are more than one independent outgoing momenta and at second order in q one must take into

account the deviation from k of the different fermion propagators.

This highlights the fundamental problem of this approach: the calculation becomes increasingly complicated when one has to expand to higher order in q. Even at this order it is not obvious how this response is invariant under small changes of the dispersion until one calculates every term by brute-force. Indeed, the topological invariance of this nonlinear response is best shown using the Green's functions directly, as done in Ref. [16]. The topological invariance of combination of Green's functions is discussed in App. B. Separating the dispersion from the eigenbasis does not help us identify the topological invariance at all.

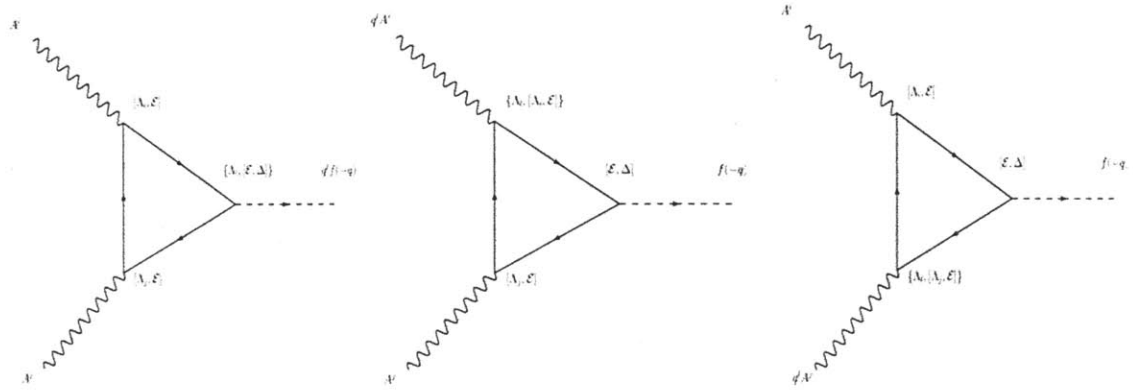


Figure 4-4: The three Feynman diagrams for 3d edge topological response.

Now we move on to three spatial dimensions. Here we would like to find the θ term as we discussed in Sec. 3.2. Similar to the calculation we have done in one spatial dimension, however, if we calculate directly to second order in the external fields, the anti-symmetrized bubble diagram is identically zero, as shown in App. E. In this formalism, we have to vary the Hamiltonian either as a function of space or time to get the effective action. We therefore insert H_δ and look for diagrams contributing at the order Λ^3. We again arrived at triangular diagrams similar to the previous example, with one A vertex replaced by H_δ. At the order of $q^1 w^1$, one needs to sum up the contribution from three diagrams, as shown in Fig. 4-4. For simplicity we also take the band to be non-dispersive. The result is

$$S_{\text{eff}} \supset S_{3D} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} i P_o \Delta P_e \Lambda^i P_o \Lambda^j P_e \Lambda^k \epsilon_{ijk} - (o \leftrightarrow e), \tag{4.30}$$

where P_o (P_e) is the projector to occupied (empty) states,

$$S_{3D} = \frac{1}{2}\int \mathrm{d}^3x\mathrm{d}t\left((\partial_t f)A_i\partial_j A_k + (\partial_i f)A_j\partial_t A_k\right)\epsilon^{ijk} \tag{4.31}$$

and recall f is the envolope function of H_δ. Using Eq. (4.20) one can show that

$$\begin{aligned}\delta P_3 &\equiv \delta(\frac{\pi}{2}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\mathrm{Tr}\left[\left(f_{ij}-\frac{1}{3}[a_i,a_j]\right)a_k)\right])\\ &= 2\pi\int\frac{\mathrm{d}^3k}{(2\pi)^3}iP_o\Delta P_e\Lambda^i P_o\Lambda^j P_e\Lambda^k\epsilon_{ijk} - (o\leftrightarrow e);\end{aligned} \tag{4.32}$$

combining, we have the effective action with variation δ:

$$S_{\text{eff}} \supset \frac{1}{4\pi}\int \mathrm{d}^3x\mathrm{d}t\left(\partial_t(\delta P_3)A_i\partial_j A_k + \partial_i(\delta P_3)A_j\partial_t A_k\right)\epsilon^{ijk}, \tag{4.33}$$

However, if one works harder and include all the diagrams that involves $\vec{\partial}\epsilon_k$, there are actually additional terms. Those terms depend on the energetics, so that it is incorrect to say the coefficient of θ term is given by P_3.

4.4 Discussion

From the results above, we know that basically in even spatial dimensions there is a bulk effective action calculable using conventional perturbative methods, whereas in odd spatial dimensions we need to vary the Hamiltonian to observe a response. This should be viewed as a problem of the method instead of a physical difference, as we clearly see the effective action in one dimension can be derived as a Berry's phase in Sec. 2.4.

Ultimately the inability for the total derivative term to show up comes from the fact that the conventional perturbation theory is perturbative in the gauge field. at any finite momentum, perturbing in the gauge field is not too different from perturbing in the field strength, providing the field strength is small enough. For responses at $q = 0$, however, perturbing in orders of the gauge field is not guaranteed to work, as the field strength then is required to be zero.

In addition to the electromagnetic sector of the effective action, one can also think about other currents and fields, such as spin currents, energy current, and Zeeman field. We can

easily extend our formalism to include these operators. For example, the energy current operator is

$$\vec{J}_E = \sum_{k,q} c^\dagger_{k+q/2} \frac{\partial H^2}{\partial \vec{k}} c_{k-q/2}, \tag{4.34}$$

and we can define the spin current to be

$$\vec{J}_{S^i} = \sum_{k,q} c^\dagger_{k+q/2} \{\sigma_i, \frac{\partial H}{\partial k}\} c_{k-q/2} \tag{4.35}$$

where σ is the Pauli matrix acting on the spin space and all internal indices are suppressed. While the energy current is derived from the conservation law, the spin current is generally not conserved unless the Hamiltonian commutes with certain spin. This definition reproduces the correct expression when the spin is conserved.

Nevertheless, it appears that it is hard to obtain any topological effective action from these currents and fields for a fermionic insulator, in the case where no spin is conserved. The energy current has an extra factor of energy, and the technical difficulty with spin arises from the fact that the spin operator in the eigenbasis is k-dependent and in general has off-diagonal matrix elements. Physically, it is just saying that in a spin non-conserving system, there is really no preferred spin direction that you can measure the topological index.

Let us consider the 2d topological insulator defined under time reversal. With the spin current defined above, we can calculate the spin current response to electric fields. The result is that in the case S^z is conserved, the response is quantized, but it is just two time-reversed copy of the integer QHE. On the other hand. if no spin is conserved, then the response is not of topological character.

Chapter 5

The Unified Formalism for Calculating Polarization, Magnetization, and More

From the discussions in previous chapters, we know we can expect topological responses in the effective theory of electromagnetic fields for a periodic insulators. As an example, the ground state polarization of a CCI insulator distinguishes between topological and trivial bands. However, we also see that there are certain difficulties to calculate the effective action using conventional perturbation methods. In this chapter, we step back, and consider the general question: how can one calculate properties such as the ground state polarization in a periodic insulator? Is there a general method which can be used to calculate similar properties to higher orders of the external fields?

5.1 A Zoo of Different Methods and their Difficulties

In recent years, there has been a series of development on how to calculate the polarization and orbital magnetization quantum-mechanically in insulating systems, in terms of Bloch wave functions.[31, 33–37] The polarization $\mathbf{P}$ measures the position differences between the band electrons and the lattice ions, which is in general nonzero in a crystal without inversion symmetry. In an open system, it results in boundary charges, which gives rise to the energy density $\Delta E = -\mathbf{P} \cdot \mathbf{E}$ in an external electric field. Inside the bulk, it is only defined modulo

ea where e is the electron charge, and a is the lattice spacing. This arises naturally from the ambiguity of associating an electron with a given ion. The reason why it has not been fully computed until rather recently is due to the unboundedness of the operator $\mathbf{r}$, which is the natural quantity to calculate the expectation value, when the lattice ions stay fixed. In Ref. [31], they overcome this problem utilizing the Wannier orbitals. The Wannier orbitals are localized in an insulating system, and the matrix elements between them are well-defined, even if the operator itself is unbounded. They also provide an alternative method, which is to compute the current response under a change of the Hamiltonian without breaking the lattice translation symmetry. The integration of the current gives the change of the polarization. This method avoids calculating $\langle \mathbf{r} \rangle$ altogether, at the expense of introducing an extra parameter and a Hamiltonian depending on it. This method also leaves the impression that only the diffrence of the polarization is properly defined. We, however, have argued otherwise in Ref. [30].

Similarly, the magnetization $\mathbf{M}$ is generally nonzero when the time-reversal symmetry is absent. The energy density change in the presence of an external magnetic field is given by $\Delta E = -\mathbf{M} \cdot \mathbf{B}$. Usually the time-reversal symmetry is broken due to magnetism, and the dominant contribution to the magnetization is of spin origin. Nevertheless, via spin-orbit coupling the orbital motion contributes to the magnetization as well. The orbital magnetization is first computed in Ref. [33, 35], either by semi-classical methods[33], or by calculating the matrix elements of $\mathbf{r} \times \mathbf{v}$ using again the Wannier orbitals.[35] In the latter work, however, special care has to be taken toward the boundary, as they show that an extra term M_{IC} arising from the "itinerent current" flowing around the boundary has to be included, in addition to the "local current" contribution M_{LC}, which involves the matrix element of $\mathbf{r} \times \mathbf{v}$ between the bulk Wannier orbitals, to give the correct and the same answer as in the former calculation. Later on in Ref. [34], the authors give a full quantum mechanical derivation, which calculates the energy of the system in a finite magnetic field based on the finite q perturbation theory of the vector potential, and taking $q \to 0$ in the end. By taking a derivative with respect to $\mathbf{B}$ one gets the magnetization $\mathbf{M}$.

After the discovery of the three-dimensional (3D) topological insulator[24, 25], it was shown in Ref. [16] via a dimensional reduction procedure from one higher dimension, that the 3D topological insulator is characterized by the θ-term, $\mathcal{L}_\theta \equiv \frac{\theta e^2}{4\pi^2} \mathbf{E} \cdot \mathbf{B}$, with $\theta = \pi$ in the effective theory, where the electrons are integrated out. With time reversal symmetry,

the coefficient θ is given by the integral of the Chern-Simons term of the Berry's connection in the Brillouin zone, which is independent of the gap size, has a 2π ambiguity, and therefore can only take the value 0 or π. In Ref. [38], it is shown that with time reversal symmetry, the θ coefficient can also be written as a Wess-Zumino-Witten- (WZW-) type term, integrated in an extended space, where one interpolates between the system in question and a trivial insulator.

Since then, there have been various attempts to calculate this term explicitly in three spatial dimensions[19, 39], without assuming time reversal symmetry. The θ-term is treated as an energy density, which can be understood as either the polarization in a magnetic field or the magnetization in an electric field, which are denoted as orbital magneto-polarizability (OMP) or orbital electro-susceptibility (OES). In Ref. [19], they offer two ways to calculate the OMP, similar to the methods described above for the polarization. In the first method they again calculate the current response to a change of Hamiltonian, but with a small uniform magnetic field turned on all the time. To perturb in the magnetic field they use the density matrix perturbation theory. In the second method, they evaluate the matrix element $\mathbf{r}$ between Wannier orbitals in the magnetic field, using the finite q perturbation theory and then take the $q \to 0$ limit. In general, however, they find that $P^i = \alpha^i_j B^j$; that is, the OMP is not diagonal, and the θ-term is just a part of it. This result is confirmed by Ref. [39], where they use the Wannier orbitals to study the OES, by calculating the magnetization in an electric field. In this calculation, similar care has to be taken on the boundary. In either calculation, the diagonal part of α^i_j is defined modulo $\frac{e^2}{2\pi}$. The easiest way to understand this physically is the following. If we consider a cylinder geometry with the material in question in the bulk, an integer quantum Hall layer on the surface of the cylinder will change the diagonal response by $\frac{ne^2}{2\pi}$, where n is the filling factor of the layer.

While all the results in the end agree with each other, the derivations are diverse, with various limitations and subtleties, as noted below:

(i) The Wannier orbitals can only be defined when the Chern number of the bands is zero.[40] Furthermore, to use the operator $\mathbf{r}$ or $\mathbf{r}\times\mathbf{v}$, one is essentially limited to settings with open boundary conditions, as they are not well-defined on a torus. The boundary then has to be treated carefully, even if we are only interested in bulk properties: in Ref. [35], to get the correct expression for the magnetization, they have to consider two contributions, M_{LC} and M_{IC} as we briefly mentioned. The first term is the usual local matrix element between

the bulk Wannier orbitals and the second term is itinerent, comes from the boundary, where the Wannier orbitals are deformed. The second term, however, can be written as a function of bulk parameters and is then argued to be present even in a setting with periodic boundary conditions. This is a subtle argument, because if we just start from the periodic system, there seems to be no reason to expect the second term. In fact, this argument reinforces that the matrix element $\mathbf{r} \times \mathbf{v}$ cannot be used to represent the magnetization $\mathbf{M}$ in a setting with periodic boundary conditions, as the M_{IC} term will be missing.

(ii) The $q \to 0$ calculation is not justified in the first place. As we know, even for free electrons, the wave function in an uniform magnetic field forms Landau levels, which are not perturbatively connected to the plane waves, in arbitrarily small magnetic fields. This is due to the fact that the perturbation is expanding in powers of $\mathbf{A}(\mathbf{q})$ in stead of $\mathbf{B}(\mathbf{q})$, where $\mathbf{B}(\mathbf{q}) = \mathbf{q} \times \mathbf{A}(\mathbf{q})$. If we do the perturbation formally anyway, in the limit $q \to 0$, but $\mathbf{B}$ remains finite, then the concern is that $\mathbf{A}(\mathbf{q})$ diverges. Indeed, in this setting we would find that the perturbed energy eigenfunctions are not orthogonal to one another at any given order. Even though the correct formulas are recovered when the $q \to 0$ limit is taken properly (probably due to the fact that we are actually calculating the physical properties at $\mathbf{B} = 0$), it is certainly desirable to have a more reliable derivation.

(iii) The method of computing the response current to an adiabatic change of the Hamiltonian can be only applied to calculate the polarization. Magnetization change, for example, does not result in any bulk current flow, and thus cannot be computed in any similar way. Another potential problem is that this method only captures the change of polarization between the two systems. It is tempting, from the point of view of this method, to claim that only the difference of the polarization is physical. While one can always define the polarization of an atomic insulator to be zero and calculate between the interpolation of that and the state in question, it is not immediately obvious that any two state with different polarization are measurably different when they are separately put with periodic boundary conditions. A derivation without referring to any other Hamiltonian is therefore desirable, as this directly shows that, for example, the polarization is an intrinsic property, independent of boundary conditions.

With the issues mentioned above in mind, we would therefore like to develop a formalism, which explains and computes everything mentioned in a unified manner. In addition, since the integer quantum Hall effect and its higher-dimensional analogs are closely related to

the quantities mentioned above and can be derived using the Green's function techniques at finite momentum, we would like to propose a formalism utilizing Green's functions. In this paper, we provide such an unified formalism. In this formalism, we do not have to work with any boundary. We can also perturb in the uniform electromagnetic fields in a gauge-invariant way, without appealing to any finite momentum calculation. All the calculations are also done without changing the Hamiltonian.

5.2 Perturbing the Green's Function in Powers of Electromagnetic Field Strengths

What are polarization and magnetization? With boundaries, they can be defined as charges and currents on the boundary; without boundaries, there has to be some inhomogeneity inside in order to observe the charges or currents. An alternative and more fundamental definition is that the polarization (magnetization) is the coefficient for the term proportional to $\mathbf{E}(\mathbf{B})$,in the effective theory, when the electrons are integrated out. The boundary and the inhomogeneity charge or currents are then naturally derived when one solves the equation of motion of the effective theory, which is just the Maxwell equations in our case.

Therefore, our goal is to do the electronic part of the path integral, in the presence of the uniform electric field and the magnetic field as a back ground, perturbatively in $\mathbf{E}$ and $\mathbf{B}$. We then have $\mathbf{P} = -\partial F/\partial \mathbf{E}$, $\mathbf{M} = -\partial F/\partial \mathbf{B}$, and $\alpha^i_j = -\partial^2 F/\partial E^i \partial B^j$, with $F = \beta^{-1} \log Z$ the free energy. This at first seems rather straight forward, as a standard diagrammatic procedure is readily available to calculate perturbative corrections to the partition function. Our goal seems no more than a one-loop calculation. It turns out not to be the case, however, when one looks carefully into the problem. The terms in the action of the effective theory we are after are total derivatives in terms of the electromagnetic gauge field. They are just zero in momentum space, where the standard procedure is carried out. This also reflects the difficulties mentioned in the previous section, as either the operator $\mathbf{r}$ or $\mathbf{r} \times \mathbf{v}$ appear in the calculation of the polarization or the magnetization exactly due to the fact that $\mathbf{E}$ and $\mathbf{B}$ are spatial derivatives of the gauge potential.

To overcome this problem, we have to calculate in position space. In addition, we have to perturb in powers of the field strength, instead of the gauge field. Let us first deal with the magnetic field. While the wave function is not perturbative in the magnetic field, as we

will show below, the gauge-invariant part of the Green's function is. The Green's function for a single-particle Hamiltonian satisfies the following equation:

$$\sum_{x'}(\omega - H)_{xx'}g_{x'x''} = \delta_{xx''}; \tag{5.1}$$

H is the single-particle Hamiltonian and g is the Green's function of the electrons. Both are n by n matrices where n labels the orbitals and spins. The system couples to a small uniform magnetic field via the Peierls substitution:

$$H_{xx'} = (H_0 + H')_{xx'}e^{\frac{ie}{\hbar}\int_x^{x'}\vec{A}\cdot dx}, \tag{5.2}$$

where H_0 is the Hamiltonian in zero field, H' is some local perturbation that is proportional to B, e.g., the atomic diamagnetism, and $\vec{A}$ is the gauge potential. Since the correction to the Green's function as well as the free energy from H' can be calculated in the standard way, we will set it to zero from now on. The line integral of the gauge potential follows a straight line from x to x'. In the following, we will use $A_{xx'}$ as the short-handed notation for $\int_x^{x'}\vec{A}\cdot dx$. We also set $e = \hbar = 1$ when there is no ambiguity. Using the idea in Ref. [41], this equation can be solved perturbatively in B in the following way:

we write

$$g_{xx'} = \tilde{g}_{xx'}e^{iA_{xx'}} \tag{5.3}$$

and notice that it does not change anything if we put $e^{iA_{xx''}}$ along with the δ-function, we get

$$\sum_{x'}(\omega - H_0)_{xx'}e^{iA_{xx'}}\tilde{g}_{x'x''}e^{iA_{x'x''}} = \delta_{xx''}e^{iA_{xx''}}. \tag{5.4}$$

Taking the exponential factor to the left-hand side, the three phases combine together, which gives the magnetic flux threading through the triangle formed by the three points x, x', x''. Independent of the gauge, we therefore have

$$\sum_{x'}(\omega - H_0)_{xx'}\tilde{g}_{x'x''}e^{iB\cdot(x'-x)\times(x''-x')/2} = \delta_{xx''}. \tag{5.5}$$

Notice that this equation is now translationally invariant, and we can solve for $\tilde{g}$ to first order in B by expanding the exponential and then Fourier transform, noting that x can be

replaced by $i\partial/\partial k$:

$$g_0^{-1}\tilde{g} - \frac{iB^c\epsilon^{abc}}{2}\frac{\partial g_0^{-1}}{\partial k^a}\frac{\partial g_0}{\partial k^b} = 1; \tag{5.6}$$

where $g_0 \equiv g_0(k) = (\omega - H_0(k))^{-1}$; $H_0(k) = \sum_x H_{0,0x}\exp(-ikx)$ and $\tilde{g}$ is in Fourier space. We therefore get

$$\tilde{g} = g_0 + \frac{iB^c\epsilon^{abc}}{2}g_0\frac{\partial g_0^{-1}}{\partial k^a}\frac{\partial g_0}{\partial k^b} + \mathcal{O}(B^2). \tag{5.7}$$

Notice that $\tilde{g}$ is gauge invariant. Once we have $\tilde{g}(k)$, the Green's function is just the inverse Fourier transform of it times the phase factor $e^{iA_{xx'}}$. We therefore have the real-space Green's function in the presence of the uniform magnetic field.

While the calculation is straightforward, to our knowledge Eq. (5.7) is a new result. In Ref. [41], without sources other than the magnetic field which breaks time reversal symmetry, this first order term vanishes and all they have to do is to set $\tilde{g} = g_0$. In that case, all the effect of the magnetic field comes from the phase.

We can extend the calculation to include the perturbative correction in the uniform electric field as well. We start from the defining equation which is the Fourier transform of Eq. (5.1):

$$(i\frac{\mathrm{d}}{\mathrm{d}t} - H)_{(x,x';t,t')}g(x',x'';t',t'') = \delta_{xx''}\delta(t-t''). \tag{5.8}$$

Now we assume the coupling to the electric field comes from the space-time extension of the Peierls phase. Note that this procedure again does not include contributions from the response of the local orbitals to the electric field. We then use the same trick, define

$$g_{xx',tt'} = \tilde{g}_{xx',tt'}e^{iA_{xx',tt'}} \tag{5.9}$$

where $A_{xx',tt'}$ is the line integral of the spacetime gauge field $(-V,\vec{A})$ on the straight line connecting the two points. Following a similar procedure, noticing that $\frac{\partial g_0^{-1}}{\partial\omega} = 1$, one can reach

$$\tilde{g} = g_0 - \frac{iE^a}{2}\big(g_0\frac{\partial g_0}{\partial k^a} - \frac{\partial g_0}{\partial k^a}g_0\big) + \mathcal{O}(E^2). \tag{5.10}$$

This procedure can easily be carried to arbitarary order of both the electric field and the magnetic field.

It is important to understand that Eq. (5.3) and Eq. (5.9) are just a way to factor out the gauge dependence of the Green's function; it is not an approximation. The only

approximation comes in when we Taylor-expand in powers of the flux threaded in the triangle formed by the three points.

Let us be concrete and give a specific example. Suppose we have a tight-binding system with n orbitals sitting on each site. The i-th orbital is located at $\vec{d_i}$ from the lattice vector $\vec{R}$. Now the Hamiltonian H_0 is an $n \times n$ matrix in momentum space, and so is $\tilde{g}$. Notice that in deriving the formula, we have implicitly chosen the gauge such that $H_0(\vec{k}+\vec{G}) = U^\dagger H_0(\vec{k})U$; U is a diagonal matrix with $U_{ii} = \exp(i\vec{G} \cdot \vec{d_i})$). The boundary condition is similar for $\tilde{g}$. Our formula is then a matrix equation for the $n \times n$ matrix $\tilde{g}$. It is important that our formula only works with this "twisted" boundary condition when there is a basis.

We note that it has been shown earlier that the one-particle density matrix (OPDM) is also perturbative in the magnetic field, and can be calculated in a similar way.[19] Many quantities we calculate below can also be calculated using the OPDM. One key difference is that the Green's function can also be perturbed in powers of the uniform electric field as we have shown above. Combining the Berry's phase procedure as we will mention later on, the Green's functions formalism is thus a truly unified framework which can calculate perturbations of the uniform electromagnetic fields to arbitrary order, including the susceptibility and polarizability. The OPDM can always be derived from the Green's functions via $\tilde{\rho}(k) = i \int \frac{d\omega}{2\pi} \tilde{g}(k)$.

At zero temperature, without the electric field, the free energy is just the expectation value of H. The path integral can thus be performed by calculating the expectation value of the Hamiltonian in a uniform magnetic field. Other perturbations in the presence of the field can be captured in the usual way, replacing fermion bilinears with the Green's functions.

With a uniform electric field, the expectation value of the Hamiltonian is no longer the same as the free energy. We can understand this fact by taking the gauge $V = 0$ (since our formulation is gauge independent.) In this gauge, the translational invariance in the time direction is lost, and one naturally does not expect any relation between the two quantities. One can directly see this by calculating the expectation value of the Hamiltonian in the presence of the electric field. We find that the expectation value of the Hamiltonian does not change with the electric field at first order.

5.3 The Berry's Phase

How do we calculate the path integral in the presence of the electric field then? The following observation provides a hint: if we think about the imaginary-time path integral, the term $\mathbf{P} \cdot \mathbf{E}$, unlike $\mathbf{M} \cdot \mathbf{B}$, stays imaginary. Indeed as we have discussed in Sec. 2.4, the polarization P^i is better thought of as a *Berry's phase*, instead of energy, when the gauge winding number in the i-direction is changed by one; i.e.

$$\phi^i_{\text{Berry}} = -2\pi P_i. \tag{5.11}$$

Similarly, the extra Berry's phase in a magnetic field is related to the OMP by

$$\Delta\phi^i_{\text{Berry}} = -2\pi\alpha_{ij}\Phi^j_B, \tag{5.12}$$

where Φ_B is the total magnetic flux threading through the system. The 2π ambiguity of both quantities thus comes naturally. For the sake of completeness, let us repeat here the procedure we have described in Sec. 2.4:

Consider a system with periodic boundary conditions. To calculate accumulated the Berry's phase during a time when, for example, $\int A_x \mathrm{d}x$ increase by 2π, first we shall consider how the single particle wave function changes as we increase A_x uniformly. The Bloch wave function is given by

$$\psi_{nk}(x) = u_{nk}(x)e^{ikx} \tag{5.13}$$

where n is a band index; $u_{nk}(x)$ is periodic and satisfies

$$\Big((\nabla - (k + A_x))^2 + V(x)\Big)\, u_{nk}(x) = E_{nk}u_{nk}(x). \tag{5.14}$$

As we increase A_x uniformly to $A_x + \eta$, the momentum k cannot change as it is fixed by the finite size L and the periodic boundary condition. On the other hand, following Eq. (5.14), $u_{nk}(x)$ changes as

$$u_{nk}(A_x + \eta) = u_{n(k-\eta)}(A_x), \tag{5.15}$$

which is just a corresponding shift of k by $-\eta$. if $\eta = 2\pi/L$, the system returns to its original

state, but in a different gauge (i.e., with winding number different by one.) Notice that while $u_{nk}(x)$ goes to the next avaiable value on the left, the k in the exponential stays the same. The electronic wave function is therefore different from its starting state. Nevertheless, if we include the gauge field, the final state differs from the initial state by a large gauge transformation, and the Berry's phase accumulated in the process is well-defined.

Now we are ready to calculate the accumulated Berry's phase of the band electrons under the process, where the winding of the gauge field in the x-direction is increased by one. Let us define $\tilde{A}_x \equiv \int \mathrm{d}x A_x$:

$$\begin{aligned}
\phi^x_{\mathrm{Berry}} &= i\int_{2\pi m}^{2\pi(m+1)} \mathrm{d}\tilde{\mathrm{A}}_{\mathrm{x}} \langle \Psi_{\mathrm{e}}| \frac{\partial}{\partial \tilde{\mathrm{A}}_{\mathrm{x}}} |\Psi_{\mathrm{e}}\rangle \\
&= i\int_{2\pi m}^{2\pi(m+1)} \mathrm{d}\tilde{A}_x \sum_{k_i, n\in \mathrm{occ}} \langle \psi_{nk_i}| \frac{\partial}{\partial \tilde{A}_x} |\psi_{nk_i}\rangle \\
&= i\sum_{k_i, n\in \mathrm{occ}} \int_{k_i}^{k_i+2\pi/L} \mathrm{d}k_x \langle u_{nk}| \frac{\partial}{\partial k_x} |u_{nk}\rangle \\
&= i\int_{\mathrm{BZ}} \mathrm{d}k \sum_{n\in \mathrm{occ}} \langle u_{nk}| \frac{\partial}{\partial k_x} |u_{nk}\rangle. \qquad (5.16)
\end{aligned}$$

$|\Psi_e\rangle$ is the total electronic wave function; in the case we are interested it is just the Slater determinant of the occupied electron wave functions at the wave vectors k_i allowed by the periodic boundary condition. In the second equality, we wrote the derivative acting on the Slater determinent as a sum of derivatives acting on single particle wave functions. In the third equality we then plug in the dependence of the wave functions, and change variables to k. Whenever $\tilde{A}_x$ increases by 2π, each u_{nk} reaches the next allowed eigenstate to the left by the periodic boundary condition (without actually changing the momentum eigenvalue.) As we sum over all the integral of eigenstates at different allowed k's, the whole Brillouin zone (BZ) is covered exactly once and we reach the fourth equality. We can read out the expression of the polarization using Eq. (5.11):

$$P^x = -i\int_{\mathrm{BZ}} \frac{\mathrm{d}k}{2\pi} \sum_{n\in \mathrm{occ}} \langle u_{nk}| \frac{\partial}{\partial k_x} |u_{nk}\rangle. \qquad (5.17)$$

This well-known result was derived in Ref. [23, 31].

How do we express the Berry's phase in terms of the Green's functions? A naive thought

would suggest that we cannot! Consider the "gauge transform" defined by

$$|u_{nk}\rangle \to \exp(i\phi(k))|u_{nk}\rangle. \tag{5.18}$$

We first observe that the Berry's phase, Eq. (5.16) is not invariant under this transform and may change by integer multiples of 2π. The Green's function, on the other hand, is clearly invariant under this gauge transform. It is therefore impossible to express the Berry's phase solely in terms of polynomials of the Green's functions. However, we then observe

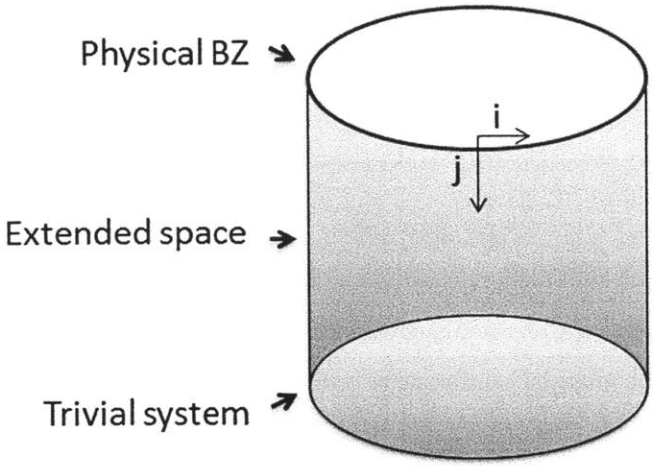


Figure 5-1: The black circle is the original physical space, with only the momentum direction along the electric field shown. The cylinder is the extended space, with the other end a trivial system. i, j are orthonormal basis on the extended space;i is along the direction of the electric field, and j points along the extra dimension.

that the Berry's phase, expressed as a gauge-dependent loop integral in momentum space, can be cast as a gauge-invariant surface integral via the Stoke's theorem. We therefore extend our system to one extra dimension in the momentum space, interpolating between the original system and a trivial system whose Berry's phase is taken to be zero.[1][38] See Fig. 1 for an illustration. The gauge dependence, then, is hidden in the way we choose to extend the wave functions. The integrand on the surface can then be expressed in terms of the Green's functions, whose definition is also extended from the circle to the cylinder.

[1]It would have looked cleaner if we can extend "to the interior"; i.e., if we can extend to a space where the Brillouin zone becomes the sole boundary. However, this procedure is problematic, when the magnetic field is not in the same direction of the electric field. The magnetic field, while uniform in the physical Brillouin zone, is no longer uniform in the extended space. By extending the space to a "cylinder" instead of a "disk", we circumvent this problem at the expense of having to introduce another boundary.

The expression is as follows:

$$\begin{aligned}\phi^i_{\text{Berry}} &= i\oint_{\partial S} \mathrm{d}k^i \sum_{\alpha\in\text{occ}} \langle u_{k\alpha}|\frac{\partial}{\partial k^i}|u_{k\alpha}\rangle \\ &= i\int_S \mathrm{d}^2\mathbf{k}\epsilon^{ij}\partial_i\langle \mathbf{u}_{\mathbf{k}\alpha}|\partial_\mathbf{j}|\mathbf{u}_{\mathbf{k}\alpha}\rangle \\ &= \frac{1}{2}\int_S \mathrm{d}^2\mathbf{k}\epsilon^{ij}\mathrm{Tr}'\left(\mathbf{g}\partial_i\mathbf{g}^{-1}\partial_j\mathbf{g}\right); \end{aligned} \tag{5.19}$$

∂S is in the i-direction, which is the direction of the electric field, and S is the enclosed cylinder in the extra dimension. Bold quantities are extended into the enclosed surface. We require that the other boundary we extend to does not contribute to the Berry's phase. The trace with prime sums over all the bands (both occupied and unoccupied), and integrates over $\omega/2\pi$ as well as the other $(d-1)$ directions perpendicular to $\mathbf{E}$. Please see App. B for a derivation.

This construction naturally separates the integral into two contributions, as discussed below: for the expression to be dependent only on the boundary variables, the integrand on the surface has to be *closed*, in differential geometry terms. It is however, not always *exact*, in that integration over a closed surface does not always give you zero. A familiar example of an integrand being closed but not exact is $\nabla\theta$ on a circle, where θ is the polar angle. It is locally a total derivative; nevertheless when you integrate it over the entire circle it gives you 2π.

We can therefore separate the integral into two contributions. The first is *exact* and can be written as a total derivative in terms of Green's functions. It thus directly becomes a boundary integral via Stokes theorem. The remaining contribution cannot be written as a boundary integral in terms of the Green's functions. However, it has to be *topological*, meaning that it is invariant under smooth deformations which vanishes on the boundary. Topological integrands are of a specific form, as we will discuss in App. B. Specifically, in d spatial dimensions the topological term is in the form of the Wess-Zumino-Witten (WZW) action[42] in $d+1$ spacetime:

$$I^d_{\text{wzw}} = \int_{\partial S} d^{d+2}x\epsilon^{a_1a_2\ldots a_{d+2}}\prod_{i=1}^{d+2}(U\frac{\partial}{\partial x^{a_i}}U^{-1}), \tag{5.20}$$

which is also defined in one extra dimensions. Our topological term will be of the same

mathematical form, with the spacetime x^{d+1} replaced by the physical momentum k^d as well as the energy ω, and the group element $U(x)$ replaced by the Green's function $g_0(k,\omega)$. Further more, the coefficient in front of the topological term is determined up to a sign by requiring that the value of the integral has a 2π ambiguity with different extension to the extended space. This point was made in Ref. [38] for the case of time reversal invariance.

Let us summarize for the formalism: we have an expression for the Green's function in the presence of an uniform magnetic field. Without the electric field, we can calculate the expectation value of the Hamiltonian to get the logarithm of the partition function. We can also calculate the charge and current responses. If we want to capture the terms linear in the electric field, however, we have to calculate a Berry's phase, which can only be expressed in terms of the Green's functions in one extra dimension. In the following section we shall see detailed calculations for all the quantities mentioned above.

5.4 Derivations for Polarization, Magnetization, and More

In this section, we show in detail how we apply the formalism given in the previous section, to three different quantities: the charge response to the magnetic field, the magnetization, and the orbital magneto-polarizability (OMP). We also discuss the θ-term, which is the isotropic part of the OMP, in higher dimensions.

5.4.1 Charge Response in a Magnetic Field

In an integer quantum Hall system in two dimensions, the magnetic field is locked with the density. This is also true for Chern insulators, which has a non-vanishing transverse conductivity in zero field. The transverse conductivity is related to the field derivative of the density by the Streda formula $\sigma_{xy} = \frac{\partial \rho}{\partial B}$. Here we first verify this result as a sanity check.

Starting from Eq. (5.7), it is straight forward to calculate the charge density in the magnetic field:

$$\begin{aligned}\langle \rho \rangle &= \frac{1}{L^2}\sum_{m,x}\langle c^\dagger_{mx} c_{mx}\rangle = i\mathrm{Tr}(g) \\ &= \int \frac{\mathrm{d}^2k}{(2\pi)^2}\frac{\mathrm{d}\omega}{2\pi} i\,\mathrm{tr}\left(g_0 + \frac{iB\epsilon^{ab}}{2} g_0 \frac{\partial g_0^{-1}}{\partial k^a}\frac{\partial g_0}{\partial k^b}\right)\end{aligned}$$

$$= \rho_0 + \frac{BC_1}{2\pi}; \tag{5.21}$$

C_1 is the Thouless-Kohmoto-Nightingale-den Nijs (TKNN) index (Chern number) of the occupied bands.[3] The capital trace in the first line implies summing over all the bands and integrating over all directions as well as energy with a facter of $(2\pi)^{-1}$ each. The lowercased trace in the second line implies summing all the bands only. The phase factor in Eq. (5.3) is absent due to the fact that the creation operator and the annihilation operator are at the same position. The last equality is derived in App. B Eq. (5.21) describes the locking of the density to the magnetic field. This "incompressibility" is fundamental to quantum Hall physics and follows from charge conservation and Faraday's law when the magnetic field is adiabatically turned on.

Nevertheless, it is somewhat intriguing to see this effect survive even on a torus with an uniform magnetic field, as our derivation implies. Without boundaries, the charge density can only change by adding or removing bulk states abruptly, even though the magnetic field is small and does not affect the energy gap in any appreciable way. In a tight-binding model, the states then must "teleport" between the occupied and empty bands. On a torus the magnetic flux has to be quantized; in the weak field limit, when we increase the magnetic flux by one flux quantum, there will be exactly C_1 states, "teleporting" from the unoccupied bands to the occupied bands, with out changing the energy gap in between. We have verified this phenomenon with a numerical diagonalization of an insulating system with $C_1 \neq 0$.

This peculiarity becomes more apparent when one compare the findings with the usual linear response derivation. There the quantized conductivity or density change is derived from a bubble diagram at finite q, in the $q \to 0$ limit. The density modulates in the same way as the magnetic field, which becomes uniform only at the limit. There are no such teleportations of the states between the bands; the electrons flows from patches with a positive magnetic field to patches with a negative magnetic field (if the Chern number is positive) and vice versa.

5.4.2 Magnetization

As sketched in the previous section, we calculate the orbital magnetization by computing the energy of the system in the presence of an uniform magnetic field, and the relation

$\mathbf{M} = -\mathrm{d}\langle H\rangle/\mathrm{d}\mathbf{B}$. We continue our derivation in two dimensions, as the magnetization is inherently a two-dimensional phenomenon. We have

$$\begin{aligned}\langle H\rangle &= \sum_{xx'}\int\frac{\mathrm{d}\omega}{2\pi}i\,\mathrm{tr}\,(H_{xx'}g_{x'x}) = \sum_{xx'}\int\frac{\mathrm{d}\omega}{2\pi}i\,\mathrm{tr}\,(H_{0xx'}\tilde{g}_{x'x})\\ &= E_0 - \frac{B\epsilon^{ab}}{2}\int\frac{\mathrm{d}^2k}{(2\pi)^2}\frac{\mathrm{d}\omega}{2\pi}\,\mathrm{tr}\left(H_0 g_0\frac{\partial g_0^{-1}}{\partial k^a}\frac{\partial g_0}{\partial k^b}\right)\end{aligned} \tag{5.22}$$

Plugging in $g_0 = \sum_m |u_m\rangle\frac{1}{\omega - E_m}\langle u_m|$ and noticing that the ω-integral restricts the poles of the two g_0's to be on opposite sides, we find that the derivative on g_0 can only act on the bra, and the derivative on g_0^{-1} can act on the bra or ket but not the energy, in order for the expression not to vanish. We can simplify the term linear in B to be

$$\begin{aligned}\langle\Delta H\rangle &= -\frac{B\epsilon^{ab}}{2}\int\frac{\mathrm{d}^2k}{(2\pi)^2}\frac{\mathrm{d}\omega}{2\pi}\sum_{m,n}\theta(-E_mE_n) \\ &\times\ \frac{E_m(E_n - E_m)}{(\omega - E_m)(\omega - E_n)}\langle u_m|\partial_a u_n\rangle\langle\partial_b u_n|u_m\rangle \\ &= \frac{iB\epsilon^{ab}}{2}\int\frac{\mathrm{d}^2k}{(2\pi)^2}\sum_{m,n}\theta(-E_mE_n) \\ &\times\ |E_m|\langle u_m|\partial_a u_n\rangle\langle\partial_b u_n|u_m\rangle.\end{aligned} \tag{5.23}$$

In the derivation we have used relations such as $\langle\partial_a u_m|u_n\rangle = -\langle u_m|\partial_a u_n\rangle$. Now we reexpress everything in terms of occupied bands only:

$$\begin{aligned}&\sum_{m,n}\theta(-E_mE_n)|E_m|\langle u_m|\partial_a u_n\rangle\langle\partial_b u_n|u_m\rangle \\ =\ &\sum_{n\in\mathrm{occ},m\in\mathrm{emp}} E_m\langle u_m|\partial_a u_n\rangle\langle\partial_b u_n|u_m\rangle \\ &-E_n\langle u_n|\partial_a u_m\rangle\langle\partial_b u_m|u_n\rangle \\ =\ &\sum_{n,n'\in\mathrm{occ}}\langle\partial_b u_n\,|H|\,\partial_a u_n\rangle\ - E_{n'}\langle u_{n'}|\partial_a u_n\rangle\langle\partial_b u_n|u_{n'}\rangle \\ &-E_n\langle\partial_a u_n|\partial_b u_n\rangle + E_n\langle\partial_a u_n|u_{n'}\rangle\langle u_{n'}|\partial_b u_n\rangle \\ =\ &\sum_{n\in\mathrm{occ}}\langle\partial_b u_n\,|H|\,\partial_a u_n\rangle\ - E_n\langle\partial_a u_n|\partial_b u_n\rangle.\end{aligned} \tag{5.24}$$

Putting Eq. (5.24) back into the expression for the energy and dividing it by B, we recover the result derived in Ref. [34, 35]:

$$M = \frac{i\epsilon^{ab}}{2} \int \frac{\mathrm{d}^2 k}{(2\pi)^2} \sum_{n \in \mathrm{occ}} \langle \partial_a u_n | H + E_n | \partial_b u_n \rangle \tag{5.25}$$

Specifically, the first term is called M_{LC} and the second term is called M_{IC} in Ref. [35]. One can also derive the same expression using the OPDM.[43].

From our derivation, both terms come together from one simple expression in the bulk. If we have a boundary, the current flowing on the edge is the sum of the two, as is required by the Maxwell equations, $\mathbf{J} = \nabla \times \mathbf{M}$. One might be tempted to conclude that the two terms generate separately measurable currents from the derivation in Ref. [35], but that is not the case. One can, however, decompose it into two contributions (different from but related to M_{LC} and M_{IC}) where the difference between the two terms can also be measured.[36]

In addition, as also discussed in Ref. [37], Eq. (5.25) naturally shows that there are C_1 gapless edge states for a Chern insulator with Chern number C_1 in two spatial dimensions. Suppose we shift the chemical potential by $\Delta\mu$. Now the magnetization changes by $C_1 \Delta\mu / 2\pi$, which implies the current on the edge changes by the same amount. If we think from the edge perspective, a chemical potential change of $\Delta\mu$ implies that the density of occupied edge states increases by $C_1 \Delta\mu / 2\pi v$, and carries additional current $C_1 \Delta\mu / 2\pi$. The two observations would not have matched, had we only taken the contribution M_{IC} as the current flowing around the edge.

On the other hand, we have the same orbital magnetization formula for a system without boundary. This means that if the system is a Chern insulator, its magnetization will depend on the chemical potential, even if there are no edges. This somewhat puzzling observation actually comes from the density locking to the magnetic field mentioned in the previous subsection. Since we define the magnetization as the derivative of the free energy with respect to B, with $F = E - \mu N$, the free energy change with the magnetic field does depend on μ. It is, however, unclear to us whether the"magnetization" defined this way is a measurable quantity on a periodic system.

With the discussions above, we therefore conclude that the magnetization of an insulator is a bulk quantity. The current flowing on the edge can always be derived via the equation of motion of the effective theory, i.e., the Maxwell equations. We also note that the orbital

magnetic susceptibility can be calculated by expanding the Green's function to second order in B.

5.4.3 Electric Polarizability

The calculation of the polarization is already covered in the previous section and in Ref.[30]. While we can express it in terms of the Green's function in one extra dimension as done in Eq. (5.19), after integrating out ω and integrating back to the boundary, the result is just what we start with. As a nontrivial example of using the formalism, here we calculate the polarizability, by considering the first order correction of the Green's function in a uniform electric field. We start from Eq. (5.19), plug in Eq. (5.10), and notice that there is an additional phase proportional to the electric field from contracting the three green's functions in real spacetime. (Notice that the time-dependent gauge potential does not break translational symmetry in the spatial direction so Eq. (5.19) still applies. The trace in the time direction, however, has to be carried out in real space; it is easier just to imagine every thing is done in real space and then converted back.) We thus have

$$\begin{aligned}
\Delta\phi^i_{\text{Berry}} &= I_1 + I_2; \\
I_1 &= \frac{iE^a}{4}\int_S \mathrm{d}^2\mathbf{k}\epsilon^{ij}\mathrm{Tr}'\Big((\mathrm{g}_0\partial_a\mathrm{g}_0 - \partial_a\mathrm{g}_0\mathrm{g}_0)\partial_i\mathrm{g}_0^{-1}\partial_j\mathrm{g}_0 \\
&+ \mathrm{g}_0\partial_i\mathrm{g}_0^{-1}\partial_j(\mathrm{g}_0\partial_a\mathrm{g}_0 - \partial_a\mathrm{g}_0\mathrm{g}_0)\Big) \\
I_2 &= -\frac{iE}{4}\int_S \mathrm{d}^2\mathbf{k}\epsilon^{ij}\mathrm{Tr}'\Big(\partial_\omega\mathrm{g}_0\partial_a\partial_i\mathrm{g}_0^{-1}\partial_j\mathrm{g}_0\Big).
\end{aligned} \tag{5.26}$$

Taking advantage of the relation $\partial_\omega \mathrm{g}_0^{-1} = 1$ and $\partial_\omega \mathrm{g}_0 = -\mathrm{g}_0^2$, we can simplify the expression to

$$\begin{aligned}
\Delta\phi^i_{\text{Berry}} &= -\frac{iE^a}{4}\int_S \mathrm{d}^2\mathbf{k}\epsilon^{ij}\mathrm{Tr}'\Big(\partial_a(\partial_\omega\mathrm{g}_0\partial_i\mathrm{g}_0\partial_j\mathrm{g}_0) \\
&+ 2\partial_i(\mathrm{g}_0\partial_a\partial_j\mathrm{g}_0)\Big) \\
&= -i\pi E^a\int\frac{\mathrm{d}\omega}{2\pi}\int_{BZ}\frac{\mathrm{d}^d k}{(2\pi)^d}\,\mathrm{tr}\big(g_0\partial_a\partial_i g_0\big).
\end{aligned} \tag{5.27}$$

Notice the only total derivative that does not vanish after integration has to be along the extra dimension. As we see here, there is no topological contribution in the polarizability;

the integral thus has to reduce to a total derivative, and we can just integrate it back to the physical Brillouin zone. Using Eq. (5.11), we get the polarizability tensor

$$\epsilon_{ij} = \frac{i}{2} \int \frac{\mathrm{d}\omega}{2\pi} \int_{BZ} \frac{\mathrm{d}^d k}{(2\pi)^d} \, \mathrm{tr}\big(g_0 \partial_i \partial_j g_0\big), \tag{5.28}$$

which is the same expression as one would get using the usual perturbation theory at finite momentum q, and take the $q \to 0$ limit.

5.4.4 Orbital Magneto-Polarizability

We can calculate the OMP by considering the polarization in a uniform magnetic field in three spatial dimensions. We start from Eq. (5.19) and plug in the Green's function in the presence of the magnetic field. Recall that i is the direction of the electric field, and j is the direction of the extra dimension:

$$\begin{aligned} \phi^i_{\text{Berry}} &= \frac{1}{2} \int_S \mathrm{d}^2\mathbf{k} \epsilon^{ij} \mathrm{Tr}' \left(\mathbf{g} \partial_i \mathbf{g}^{-1} \partial_j \mathbf{g}\right) \\ &\equiv 2\pi^2 \epsilon^{ij} L^2 \mathrm{Tr}^S \left(\mathbf{g} \partial_i \mathbf{g}^{-1} \partial_j \mathbf{g}\right) \end{aligned} \tag{5.29}$$

Here $\mathbf{g}$ denotes the Green's function at a given momentum in the (i,j) surface. It is in general not translationally invariant in the remaining directions. Here we introduce the new notation Tr^S for later convenience. Tr^S is defined as integrating over momentum divided by $(2\pi)^2$ in the (i,j) direction within the boundary, integrating over $\omega/2\pi$, and summing over positions, divided by L in the remaining directions if they are not translationally invariant; the lattice is replaced by integration over the momentum and divided by (2π) otherwise. When $\mathbf{E}$ and $\mathbf{B}$ are not perpendicular, we have to take a Landau gauge to make the Green's function translationally invariant in the direction of the electric field for the derivation in the previous section to work; it nevertheless does not affect the result, Eq. (5.29), and our calculation below.

Now we plug in Eq. (5.7). To first order in $\mathbf{B}$, not only do we have $\tilde{\mathbf{g}}$ to first order, but we also have to consider that the three product of $\mathbf{g}$'s, contains three phases which sums to be the flux threading through the triangle. Indentical to what we did in Sec. II, we Fourier transform, Taylor-expanding the phase to first order in $\mathbf{B}$. The result is

$$
\begin{aligned}
\Delta\phi^i_{\text{Berry}} &= I_1 + I_2; \\
I_1 &= \pi^2 i B^c L^2 \epsilon^{abc}\epsilon^{ij}\mathrm{Tr}^S\big(\mathbf{g}_0\partial_a\mathbf{g}_0^{-1}\partial_b\mathbf{g}_0\partial_i\mathbf{g}_0^{-1}\partial_j\mathbf{g}_0 \\
&+ \mathbf{g}_0\partial_i\mathbf{g}_0^{-1}\partial_j(\mathbf{g}_0\partial_a\mathbf{g}_0^{-1}\partial_b\mathbf{g}_0)\big) \\
I_2 &= -\pi^2 i B^c L^2 \epsilon^{abc}\epsilon^{ij}\mathrm{Tr}^S\left(\partial_a\mathbf{g}_0\partial_b\partial_i\mathbf{g}_0^{-1}\partial_j\mathbf{g}_0\right);
\end{aligned}
\tag{5.30}
$$

I_1 is from first-order terms in $\tilde{\mathbf{g}}$ and I_2 is from the phase. $\mathbf{g_0}$ is the Green's function in zero magnetic field in the extended space. The trace now indicates integration in all the momentum directions as well as ω and divided by (2π) in each direction, as the translational invariance is restored. I_1 can be rewritten as

$$
\begin{aligned}
I_1 &= \pi^2 i B^c L^2 \epsilon^{abc}\epsilon^{ij}\mathrm{Tr}^S\big(\mathbf{g}_0\partial_a\mathbf{g}_0^{-1}\partial_b\mathbf{g}_0\partial_i\mathbf{g}_0^{-1}\partial_j\mathbf{g}_0 \\
&+ (i\leftrightarrow a, j\leftrightarrow b) - \partial_j(\partial_i\mathbf{g}_0\partial_a\mathbf{g}_0^{-1}\partial_b\mathbf{g}_0)\big)
\end{aligned}
\tag{5.31}
$$

in which the last term in the second line can readily be integrated back to the physical momentum space. The first two terms are almost in the form of the topological terms we mentioned in App. B, but without complete antisymmetrization among the indices.

Let us now look at I_2. We would like to separate this term into a total-derivative and some remaining parts which give the topological term; to achieve this, we need to take advantage of the condition $\partial_\omega\mathbf{g}_0^{-1} = 1$. Note that this relation also implies $\partial_\omega\partial_a\mathbf{g}_0^{-1} = 0$ and $\partial_\omega\mathbf{g}_0 = -\mathbf{g}_0^2$. By inserting $\partial_\omega\mathbf{g}_0^{-1}$ at the end of the term and integrating the ω-integral by parts, we find (from here on we omit the subscript of $\mathbf{g}_0$ to avoid cluttering in the equations):

$$
\begin{aligned}
0 &= \mathrm{Tr}^S\Big(\mathbf{g}\partial_a\mathbf{g}^{-1}\mathbf{g}(\partial_b\partial_i\mathbf{g}^{-1})\mathbf{g}\partial_j\mathbf{g}^{-1}\mathbf{g} \\
&+ \mathbf{g}(\partial_b\partial_i\mathbf{g}^{-1})\mathbf{g}\partial_j\mathbf{g}^{-1}\mathbf{g}\partial_a\mathbf{g}^{-1}\mathbf{g} \\
&+ \mathbf{g}\partial_j\mathbf{g}^{-1}\mathbf{g}\partial_a\mathbf{g}^{-1}\mathbf{g}(\partial_b\partial_i\mathbf{g}^{-1})\mathbf{g}\Big).
\end{aligned}
\tag{5.32}
$$

For convenience, we use the notation $(\mathbf{abij})$ to stand for $\mathrm{Tr}^S(\mathbf{g}\partial_a\mathbf{g}^{-1}\mathbf{g}\partial_b\mathbf{g}^{-1}\mathbf{g}\partial_i\mathbf{g}^{-1}\mathbf{g}\partial_j\mathbf{g}^{-1}\mathbf{g})$,

$(\mathbf{a[bi]j})$ to stand for $\mathrm{Tr}^S(\mathbf{g}\partial_a\mathbf{g}^{-1}\mathbf{g}(\partial_b\partial_i\mathbf{g}^{-1})\mathbf{g}\partial_j\mathbf{g}^{-1}\mathbf{g})$, ..., etc. The equation above becomes

$$(\mathbf{a[bi]j}) + (\mathbf{[bi]ja}) + (\mathbf{ja[bi]}) = 0. \tag{5.33}$$

Also, Eq. (5.31) becomes

$$(\mathbf{abij}) + (\mathbf{ijab}) - \partial_\mathbf{j}(\mathbf{iab}); \tag{5.34}$$

We then integrate by parts twice on the second and the third term, noticing that a, b and i, j are separately antisymmetrized, to make them into the form of the first:

$$\begin{aligned}
(\mathbf{[bi]ja}) &= (\mathbf{a[bi]j}) + (\mathbf{ibja}) - (\mathbf{bjia}) + \partial_\mathbf{i}(\mathbf{bja}); & (5.35)\\
(\mathbf{ja[bi]}) &= (\mathbf{a[bi]j}) + (\mathbf{jaib}) - (\mathbf{jbai}) - \partial_\mathbf{j}(\mathbf{bai}). & (5.36)
\end{aligned}$$

We therefore have

$$\begin{aligned}
-(\mathbf{a[bi]j}) &= \frac{1}{3}\big(-(\mathbf{bjia}) - (\mathbf{jbai}) + (\mathbf{ibja}) + (\mathbf{jaib})\\
&+ \partial_\mathbf{i}(\mathbf{bja}) - \partial_\mathbf{j}(\mathbf{bai})\big). \qquad (5.37)
\end{aligned}$$

Now we can sum over all contributions, and get

$$\begin{aligned}
\Delta\phi^i_{\mathrm{Berry}} &= \pi^2 i B^c L^2 \epsilon^{abc}\epsilon^{ij}\Big((\mathbf{abij}) + (\mathbf{ijab})\\
&+ \frac{1}{3}\big((\mathbf{bija}) + (\mathbf{jabi}) + (\mathbf{ibja}) + (\mathbf{jaib})\big)\\
&- \partial_\mathbf{j}(\mathbf{iab}) + \frac{1}{3}\big(\partial_\mathbf{i}(\mathbf{bja}) - \partial_\mathbf{j}(\mathbf{bai})\big)\Big) \qquad (5.38)
\end{aligned}$$

Notice that the integrating-by-part trick in the ω-direction can also be applied to expressions such as $(\mathbf{abij})$ and $(\mathbf{iab})$, and similarly we get

$$\begin{aligned}
(\mathbf{abij}) + (\mathbf{bija}) + (\mathbf{ijab}) + (\mathbf{jabi}) &= 0 & (5.39)\\
(\mathbf{aibj}) + (\mathbf{ibja}) &= 0 & (5.40)\\
(\mathbf{iab}) + (\mathbf{abi}) + (\mathbf{bia}) &= 0 & (5.41)
\end{aligned}$$

Therefore, by writing

$$(\mathbf{abij}) + (\mathbf{ijab}) = \frac{1}{3}\left((\mathbf{abij}) + (\mathbf{ijab}))\right) - \frac{2}{3}\left((\mathbf{bija}) + (\mathbf{jabi})\right), \tag{5.42}$$

the "topological part" of ϕ_{Berry} is

$$\Delta\phi^i_{\text{Berry,wzw}} = \frac{1}{3}\pi^2 i B^c L^2 \epsilon^{abc}\epsilon^{ij}\Big((\mathbf{abij}) + (\mathbf{ijab}) + (\mathbf{aijb}) + (\mathbf{iabj}) + (\mathbf{ibja}) + (\mathbf{ajbi})\Big). \tag{5.43}$$

Notice that this term is totally antisymmetric in all the indices. This is expected, as it is topological only when all the indices are antisymmetrized. It is also of the form of the WZW action if we put $\partial_\omega g^{-1}$ into the expression.

Since the direction of the magnetic field is perpendicular to the (ab) plane, it has to be in the (ij) plane, for the topological term not to vanish. This implies that only the component of the magnetic field in the direction of the electric field contributes in the topological part. Gathering everything we finally have

$$\Delta\phi^i_{\text{Berry,wzw}} = \frac{\pi^2 i}{3}\Phi^i_B\epsilon^{abcd}(\mathbf{abcd}) \tag{5.44}$$

The remaining part can be reorganized using Eq. (5.41):

$$\Delta\phi^i_{\text{Berry,3d}} = -\frac{2\pi^2 i}{3}\Phi^c_B\epsilon^{abc}\epsilon^{ij}\big(\partial_{\mathbf{j}}(\mathbf{bai}) + \partial_{\mathbf{j}}(\mathbf{iab})\big) \tag{5.45}$$

Integrating back to the physical momentum space, we have

$$\Delta\phi^i_{\text{Berry,3d}} = \frac{\pi i}{3}\Phi^c_B\epsilon^{abc}\big((iab) + (bai)\big). \tag{5.46}$$

Here (iab) stands for $\text{Tr}\big(g\partial_i g^{-1} g\partial_a g^{-1} g\partial_b g^{-1} g\big)$ with the trace summing over the energy as well as the physical momentum directions, with $(2\pi)^{-1}$ in every direction. The difference of a factor of (2π) in front comes from the different number of $(2\pi)^{-1}$ in the definition of the traces Tr^S and Tr, in four and three spatial dimensions respectively. Combining, we thus

have our final answer in terms of the Green's functions:

$$\begin{aligned}
\alpha_{ij} &= (\alpha_{\rm wzw} + \alpha_{\rm 3d})_{ij}, \\
\alpha_{{\rm wzw}ij} &= -\frac{\pi i}{6}\epsilon_{abcd}{\rm Tr}^S({\rm g}\partial_a{\rm g}^{-1}{\rm g}\partial_b{\rm g}^{-1}{\rm g}\partial_c{\rm g}^{-1}{\rm g}\partial_d{\rm g}^{-1}{\rm g})\delta_{ij}; \\
\alpha_{{\rm 3d}ij} &= -\frac{i}{6}\epsilon_{abj}{\rm Tr}\big(g\partial_i g^{-1}g\partial_a g^{-1}g\partial_b g^{-1}g - h.c.\big).
\end{aligned} \tag{5.47}$$

Notice that in terms of the Green's functions, $\alpha_{\rm wzw}$ can only be expressed with the extended dimension. Eq. (6.2) generalizes the result in Ref. [38] to the generic time-reversal breaking cases, where the WZW integral can take continuous values. Note that there is an additional term $\alpha_{\rm 3d}$ which is zero in the time reversal invariant case.

To get the expression entirely in terms of variables in the physical momentum space, we have to expand the Green's functions explicitly in the eigenbasis then integrate it back to the physical momentum space. Taking advantage of the topological property of $\alpha_{\rm wzw}$ and using Eq. (B.9) in App. B, we can immediately know that the first term contains a part which can be expressed using the Berry's phase gauge field strength, and some other part which is a global total derivative, and invariant under the gauge transform defined by Eq. (5.18). When integrated back to the physical momentum space, the first part becomes the Chern-Simons term with the Berry's phase gauge field $\mathcal{A}_{\mu,nn'} \equiv \langle u_{nk}| - i\frac{\partial}{\partial k^\mu}|u_{n'k}\rangle$; the remaining part combined with $\alpha_{\rm 3d}$ gives the rest of the tensor α_{ij} as derived in Ref. [19]:

$$\begin{aligned}
\alpha_{ij} &= (\alpha_{\rm CS} + \alpha_{\rm G})_{ij}; \\
\alpha_{{\rm CS}ij} &= -\frac{1}{2}\delta_{ij}\int\frac{{\rm d}^3k}{(2\pi)^3}\epsilon^{abc}{\rm tr}(\mathcal{A}_a\partial_b\mathcal{A}_c + i\frac{2}{3}\mathcal{A}_a\mathcal{A}_b\mathcal{A}_c); \\
\alpha_{Gij} &= \frac{1}{2}\epsilon_{abj}\int\frac{{\rm d}^3k}{(2\pi)^3}\sum_{m\in{\rm emp},n\in{\rm occ}}\Bigg(\\
&\qquad \frac{\langle\partial_i n|m\rangle\,\langle m\,|\{\partial_a H,\partial_b\mathcal{P}\}|\,n\rangle}{E_n - E_m} + c.c.\Bigg),
\end{aligned} \tag{5.48}$$

where $\mathcal{P} \equiv \sum_{n\in{\rm occ}}|n\rangle\langle n|$ is the projector to the occupied bands. The detail of the calculation is shown in App. C. A similar calculation performed using the density matrix perturbation theory is provided in App. D.

5.4.5 θ-term in higher dimensions

While it is straight forward to generalize the complete calculation in the previous section to obtain all components of the anolog of OMP in higher dimensions, the totally-antisymmetric part, i.e., the θ-term, is especially easy to compute. Here as an illustration, we calculate the coefficient $\theta_{5\mathrm{d}}$ of the θ-term in (5+1)D as defined below:

$$\mathcal{L}_\theta = \frac{\theta_{5\mathrm{d}}}{384\pi^3}\epsilon^{\alpha\beta\gamma\delta\mu\nu}F_{\alpha\beta}F_{\gamma\delta}F_{\mu\nu}. \tag{5.49}$$

First we find the Green's function to second order of the magnetic field. In higher dimensions, the term in the exponential in Eq. (5.5) becomes $[iF_{ab}(x'-x)^a(x''-x)^b/2]$. Since we are only interested in contributions with all the indices antisymmetrized, only first derivatives will contribute. When we Taylor-expand Eq. (5.5) to second order and Fourier transform, we get

$$\begin{aligned}\tilde{g}_2 &= -\frac{1}{4}(F_{ab}F_{cd}+F_{ad}F_{bc}+F_{ac}F_{db}) \\ &\quad g_0(\partial_a g_0^{-1})g_0(\partial_b g_0^{-1})g_0(\partial_c g_0^{-1})g_0(\partial_d g_0^{-1})g_0+\ldots,\end{aligned} \tag{5.50}$$

where $\tilde{g}_2$ is the second order term of $\tilde{g}$, and the indices run through all five spatial directions. The $(\ldots)$ vanishes when we antisymmetrize all the indices. Plugging into Eq. (5.19), we then have

$$\begin{aligned}\phi^i_{\mathrm{Berry}} &= -\frac{3\pi^2}{2}\epsilon^{ij}L^4(F_{ab}F_{cd}+F_{ad}F_{bc}+F_{ac}F_{db}) \\ &\quad (\mathbf{ijabcd})+\ldots,\end{aligned} \tag{5.51}$$

where we have used the abbreviated notation introduced in the previous section. We still only need to keep track of the parts which do not vanish after antisymmetrizing all the indices. Antisymmetrizing, noticing that in each direction (say E_x, B_{yz}, B_{uv}) summing over indices gives a factor of 8, we then have

$$\phi^{\mathrm{iso}}_{\mathrm{Berry}} = -\frac{\pi^2}{60}\epsilon^{abcdef}(\mathbf{abcdef})\Phi^1_B\Phi^2_B, \tag{5.52}$$

Φ^1_B and Φ^2_B are the two magnetic fluxes threading through the four directions prependicular to the electric field. Notice that from the definition Eq. (5.49), $\theta_{5\mathrm{d}}$ is exactly the Berry's

phase when the flux threading through each direction equals 2π, we then have

$$\begin{aligned} \theta_{5d} &= -\frac{\pi^4}{15}\epsilon^{abcdef}(\mathbf{abcdef}) \\ &= -\frac{1}{1920\pi^3}I_F^6; \end{aligned} \tag{5.53}$$

I_F^6 is defined in Eq. (B.6). This is the higher-dimensional analog of the trace of α_{wzw}, which includes both the second Chern-Simons term $\mathcal{A}\wedge\mathcal{F}\wedge\mathcal{F}$, and some other inter-gap contributions. To reexpress θ_{5d} entirely in terms of Bloch wave functions and energies in the physical Brillouin zone, however, is rather tedious, and we shall not do it here.

5.5 Discussion

In this chapter, we provide a formalism to integrate out the electrons with external uniform electromagnetic fields. This formalism provides a unified and systematic way to calculate quantum-Hall type responses, polarization, polarizability, orbital magnetization, orbital magnetic susceptibility, and OMP. From the perspective of the formalism, all of the quantities mentioned are of bulk nature, and all calculations can be done with periodic boundary conditions. The existence of the edge current or response can be derived from the equation of motion of the resulting effective theory, which is defined in the bulk, independent of the boundary conditions.

In our formulation, one key insight is that the linear term in the magnetic field is an energy, whereas the linear term in the electric field contains a Berry's phase. This explains why the polarization and the OMP are defined only modulo 2π in certain units, whereas the magnetization is always rigorously defined.

The wave function under an uniform magnetic field is nonperturbative; nevertheless, the gauge invariant part of the Green's function is perturbative, even strictly at $q = 0$. In Eq. (5.7), the only expansion parameter is the flux enclosed in the triangle; inside an insulator with finite range correlation functions, the expansion is controlled.

When the θ-term is first discovered in the 3D topological insulators, it was shown for time-reversal invariant systems, θ is given by the Chern-Simons term of the Berry's phase gauge field defined in momentum space. It is not until much later that extra contributions which depend on the inter-gap matrix elements as well as the gap size are discovered for

the general case without time reversal invariance, along with the off-diagonal components. From our calculation, two terms come together naturally, and are most simply expressed as an integral of the WZW term with Green's functions in the extended space. The same conclusion holds for the higher dimensional θ term as well.

However, we have to note that it is not easy to convert the expression in the extended space back to the Bloch wave functions and energies in the physical Brillouin zone. For this purpose, the density matrix perturbation theory formalism[30] seems to be more useful. Nevertheless, from those methods it is harder to obtain the Chern-Simons term; it is also not as straight-forward to generalize to higher dimensions. Our formula Eq. (6.2) and the higher dimensional generalization Eq. (5.53) thus complement the other methods and offer a better conceptual understanding.

There is an important difference between the derivation of the θ-term using our approach and the dimensional reduction procedure used in Refs. [16, 38], as we summarized in Sec. 1.3.2. Even though they give the same result with time reversal symmetry, the latter is not readily generalizable to the general case without time reversal symmetry.

Chapter 6

Dependence of Bulk Physics on the Boundary

We now have seen how one can systematically derive the bulk effective action with periodic boundary conditions. We see that there are properties which are like phases, such as the orbital magnetic polarizability, are defined only modulo 2π in proper units. With a boundary, however, those quantities are further determined by the details at the boundary.

We thus come through a full circle. The topology of the bands manifests itself through the edge states. We try to understand it without the edges and we have got a bulk effective description. Does the description change with different boundary conditions?

In this chapter, we will discuss how various bulk quantities can depend on the boundaries, based on how they are calculated in the previous chapter. In particular, we will show that when the calculation with periodic boundary conditions does not involve a Berry's phase, the quantity in question is determined unambiguously by the bulk, even in the presence of gapless surface states. When the calculation involves a Berry's phase, the bulk can only determine the quantity up to some quantized value, given that (i) there are no gapless surface states, (ii) the surfaces do not break the symmetries preserved by the bulk, and (iii) the system is kept at charge neutrality. If any of the above conditions is violated, the quantity is then determined entirely by the details at the boundary. Due to the strong dependence on the boundary, this kind of thermodynamic quantity, such as the isotropic magneto-electric coefficient, cannot be measured in the bulk without careful control at the boundary.

In the following, we will discuss case by case from the ground state polarization, orbital magnetization, to the magneto-electric tensor. We will argue through Gedanken experiments that some of them depends on the boundary while others don't. We will verify our argument with numerical simulations. By matching the observations with our previous calculation done with periodic boundary conditions, we can then directly tell from the calculation with periodic boundary conditions how different thermodynamic quantities depend on boundaries.

6.1 Ground state polarization

The ground state polarization is given by the following formula with periodic boundary conditions:[31]

$$P = -ie \int_{BZ} \frac{\mathrm{d}^d k}{2\pi^d} \sum_{\alpha(k)\in occ} \langle \alpha(k) | \frac{\partial}{\partial k} | \alpha(k) \rangle. \tag{6.1}$$

In one spatial dimension (1d), the polarization is defined modulo e with periodic boundary conditions: $P = P_0 + ne$, with n an integer. This corresponds to the observation that with periodic boundary conditions, we can move every electron to the next unit cell and return to the original state, while the two states should by definition have polarization differed by e. With two ends, the polarization will take one specific value, depending on the number of charges we put at the two ends.

However, if there are zero modes at the two ends, the polarization is then ambiguous, as theoretically we can consider superposition of states of different occupancy of the zero modes. The bulk value of the polarization thus depends entirely on the boundary.

In 3d it is a bit more interesting. For simplicity let us assume the system sits on a cubic lattice of size a. Now the bulk formula has an ambiguity of e/a^2, which also corresponds well to the fact that we can move every electron to the next unit cell and return to the same state. However, with boundary surfaces the situation becomes quite different. Consider a capacitor setup. We are allowed to put any number of charges on each of the opposing surfaces, resulting in a change of the polarization in units of e/A (A is the total surface area). In the thermodynamic limit, we can put any finite density of charges on the surface, and the polarization in the bulk can take any value. Our bulk formula is thus no longer valid. To accommodate the charge on the surface, however, the system needs to either be

in a metallic state near the boundary, or to break the lattice translation symmetry in the two in-plane directions. If neither condition is satisfied, then we can only add an integer number of electrons per unit cell, and the bulk formula is recovered, with the remaining ambiguity determined by the surface.

How can the bulk formula become invalid? We note that the ground state polarization can be understood as a Berry's phase when one adiabatically turns on the electric field. Firstly, in order for the Berry's phase to make any sense, the system has to be gapped. This is the reason why a metallic surface can render the bulk formula invalid. Secondly, if we break the lattice translation symmetry in the two directions perpendicular to the electric field, we can no longer integrate over the momentum in those directions but should instead sum over a large number of sub-bands labelled by the remaining momentum along the direction of the electric field. The polarization will have an ambiguity of e/A in this case. This is different from the conventional thermodynamic quantity, which will require a symmetry breaking in the bulk to change its value. The Berry's phase is thus a rather fragile thermodynamic quantity.

6.2 Ground state orbital magnetization

It is not immediately obvious that the orbital magnetization is independent of the boundary. In the bulk the operator $\hat{M} \propto (\mathbf{r} \times \mathbf{v})$ is ill-defined with periodic boundary conditions, and seems to be growing as one goes near the boundary. Indeed, when one numerically compute $\langle \hat{M} \rangle$ summing over the local orbitals, there is a finite contribution from the boundary orbitals, which renders the total orbital magnetization different from the naive bulk value. [37] Nevertheless, it has been shown[37] that the boundary contribution is in fact independent of the details at the boundary via the use of local Wannier functions, in an insulator with zero Chern number.

However, in a Chern insulator, a local Wannier function can not be found[40, 44], because the Bloch functions cannot be periodic and smoothly defined over the Brillouin Zone. To see that even in this case the orbital magnetization is still independent of the boundaries, we can consider the following setup:

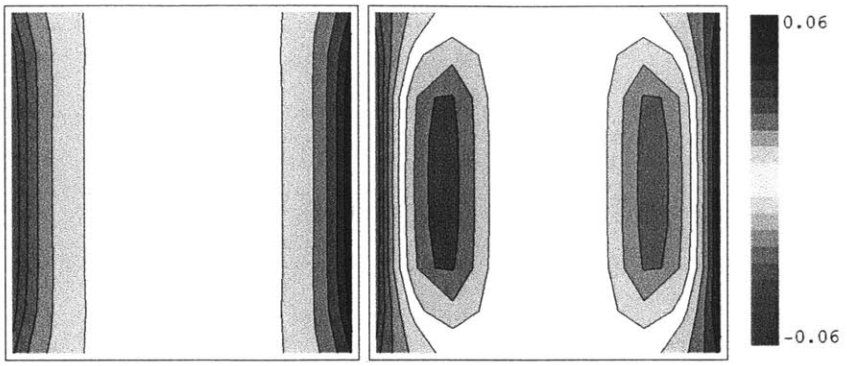
Suppose we have an insulator with a non-vanishing Chern number in two dimensions. Let us imagine putting an auxiliary layer of insulator on top, with an opposite Chern number,

without any interaction with the original one. The new insulator as a whole is then of total Chern number zero. We can therefore make a local Wannier orbital, by a linear combination of orbitals from the two layers.[45] The argument then goes through for the insulator as a whole, and the total orbital magnetization should be independent of the boundary. Now since there is no interaction between the two layers, the total magnetization is just the sum of the magnetization of the original insulator and the auxiliary insulator. We now consider a particular boundary condition, where the two insulators couples to independent boundary terms that do not interact with each other as well. Let us only vary the boundary terms that couple to the original insulator. The total magnetization cannot change, and neither the contribution from the auxiliary insulator. We thus have to conclude that even for a Chern insulator, the orbital magnetization is independent of the boundaries.

From this abstract point of view, the generalization to Chern insulators seems rather trivial. However, the presence of gapless chiral edge states may cause one to worry. Suppose we can gate the material to supply a constant chemical potential, what will happen if we turn up the electric potential on the edge? Will the edge current decrease because fewer edge states are occupied, or will it stays the same as required for the bulk magnetization not to change?

We do a straightforward numerical simulation to resolve this paradox. The result is shown in Fig. 6-1. We can see that while shifting the overall chemical potential creates circulating currents, altering the electric potential locally at the edge does not change the bulk magnetization. If we look closer, while the current right at the edge is changed, there is a counter-propagating current near the edge, which keeps the total current localized near one edge constant. The counter-propagating current is just the integer quantum Hall response to the electric potential gradient. This bulk quantum Hall current exactly compensates for the current carried by the now-unoccupied edge states, and leaves the bulk magnetization insensitive to the change of the potential local near the edge.

A very similar puzzle arises in the S_z conserved spin Hall insulator. On the edge there are counter-propagating TR-paired edge states. When we apply a uniform Zeeman field H_z, there will be a net circulating current from the edge states. We can therefore deduce a bulk orbital magnetization response to the Zeeman field. We call this the orbital-Zeeman susceptibility. However, one can locally break the S_z conservation together with the TR symmetry near the edge, to gap out the edge states. In this case, will there still be a bulk



(a) (b)

Figure 6-1: We take our Hamiltonian to be $H = \sum_n c_n^\dagger(\tau_z - i\tau_x)c_{n+\hat{x}} + c_n^\dagger(\tau_z - i\tau_y)c_{n+\hat{y}} + mc_n^\dagger\tau_z c_n + h.c.$, where $\tau's$ are the Pauli matrices. At half filling with $m = 1.5$, the band carries a Chern number $C_1 = 1$. If we set the chemical potential $\mu = 0$, the ground state has no magnetization. We put the Hamiltonian on a 10×10 lattice, and take open boundary conditions in both directions. The current on the vertical links is plotted. We relate the current to the magnetization by $I^b = \epsilon^{ab}\partial_a M$, and take the magnetization at the middle to represent the bulk magnetization. (a) $\mu = 0.5$. As expected, some edge states are occupied and give rise to a bulk magnetization. (b) If we set $\mu = 0$ but locally apply an electric potential $V = -0.5$ to the first two rows at the boundary, the edge states are again occupied. However, in the region next to those layers, a counter-propagating current takes place. The bulk magnetization remains zero (barring some finite size effect).

magnetization response to the Zeeman field?

The numerical result is shown in Fig. 6-2. Here we can see that even though the edge states are gapped out by the local perturbations, the total current flowing near the edge remains the same. The local perturbation transfers the current from the states at the Fermi level, to the occupied bands. In the end, while local properties can affect the gapless states, the total current near the edge in the is unaffected.

We therefore conclude that the orbital magnetization, as well as the orbital-Zeeman susceptibility is independent of the boundary for an insulator. While the circulating current may be carried by the edge states, the total amount is entirely insensitive to the local boundary conditions. One can understand this from a calculation with periodic boundary conditions: the magnetization is calculated as an energy density in a magnetic field. The total energy, unlike the Berry's phase, is a truly extensive property, so that the boundary contribution is irrelevant in the thermodynamic limit. The energy density in the bulk is thus entirely independent of the boundaries far away enough, whether there are gapless states or not.

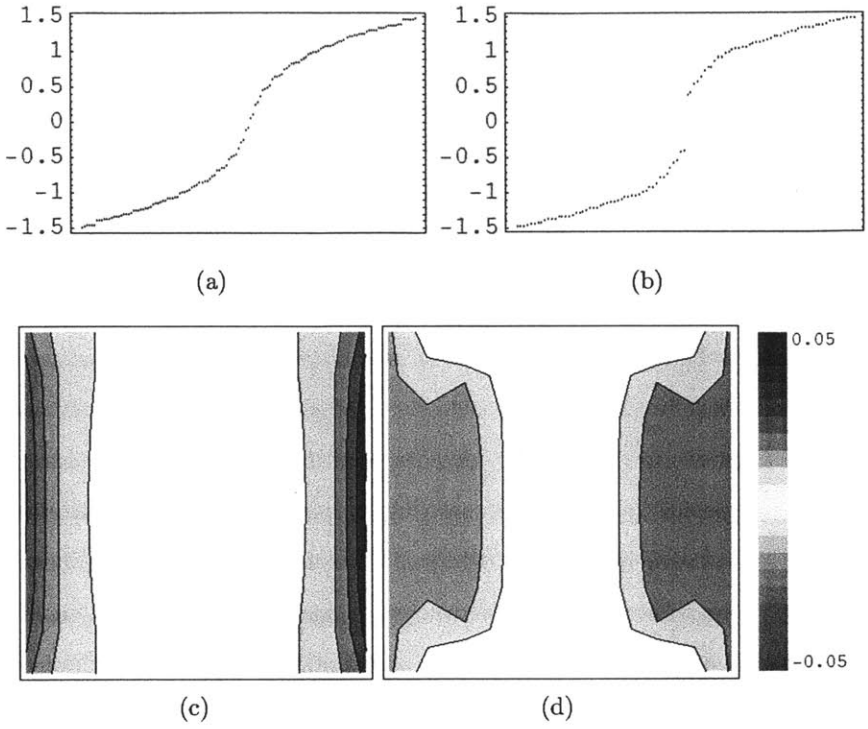


Figure 6-2: We now think of the previous model as from spin up electrons and pair it with its time reversal. We applied a unifrom Zeeman field $\delta H_z = 0.2\sum_n c_n^\dagger S_z c_n$. (a) We plot the eigenstate energies in ascending order. The edge states live inside the gap. (b) By applying a time-reversal as well as S_z symmetry breaking term near the boundary $\delta H = \sum_{\mathrm{n}\in\mathrm{edge}} c_n^\dagger S_x c_n$, we can gap out the edge states. (c)-(d) We look at the current on the vertical links. While the current distributes slightly differently with or without the symmetry breaking term at the edges, the contributions to the bulk magnetization are identical.

6.3 Magneto-electric Effect

After the discussion of the polarization and the magnetization and seeing that they are thermodynamic quantities with very different behaviors, it is thus a natural question to ask the same question about the ME tensor; in addition, about how the Maxwell relation can be maintained. Before going into details of the boundary dependence, however, let us first show that the anisotropic part α_{3d} is independent of the boundaries.

In terms of electronic Green's functions and with periodic boundary conditions, we have derived the ME tensor from the OMP perspective, as a Berry's phase in a magnetic field:[46]

$$\alpha_{ij} = (\alpha_{\mathrm{wzw}} + \alpha_{\mathrm{3d}})_{ij},$$

$$\begin{aligned}\alpha_{\mathrm{wzw}ij} &= -\frac{\pi i}{6}\epsilon_{abcd}\mathrm{Tr}^S(\mathbf{g}\partial_a\mathbf{g}^{-1}\mathbf{g}\partial_b\mathbf{g}^{-1}\mathbf{g}\partial_c\mathbf{g}^{-1}\mathbf{g}\partial_d\mathbf{g}^{-1}\mathbf{g})\delta_{ij};\\ \alpha_{\mathrm{3d}ij} &= -\frac{i}{6}\epsilon_{abj}\mathrm{Tr}(g\partial_i g^{-1}g\partial_a g^{-1}g\partial_b g^{-1}g - h.c.).\end{aligned} \tag{6.2}$$

The traces include the frequency and momentum integral divided by factors of (2π); the symbol Tr^S denotes the integral and trace in one extra dimension in momentum space, with the original Brillouin zone and a trivial test system as the boundary. While the entire ME tensor is derived as a Berry's phase, α_{3d} does not depend on the Green's function extended to the extra dimension. Without considering boundaries directly, we can show that α_{3d} is independent of the boundaries, by showing it extends smoothly to finite frequency and momentum.

At finite frequency and momentum, the ME response is understood as a term in the effective action which is proportional to $E^i(q,\omega)B^j(-q,-\omega)$. Unlike the uniform ME response however, this term can no longer be understood as OMP or OES, due to the fact that unlike uniform electromagnetic fields, the electric and magnetic fields at finite frequency and momentum are related by Faraday's law. The term nevertheless affects properties of the propagating electromagnetic waves. For our purposes, it suffices to show that the effective Lagrangian is continuous from $q = 0$ to $q \to 0$. At any $q \neq 0$, we can calculate the effective Lagrangian by the conventional diagrammatic method. Calculated in App. E, the bubble diagram gives

$$S_{ME} = -\int \frac{\mathrm{d}^4 q}{(2\pi)^4} B^\ell(q)E^k(-q)\alpha_{\mathrm{3d}k\ell} + \mathcal{O}(q). \tag{6.3}$$

Comparing with Eq. (6.2), we see that α_{3d} is continuous, whereas α_{wzw} is entirely absent at finite momentum. One might worry that we have missed α_{wzw} in momentum space due to the fact that it is a total derivative in real space, which Fourier transforms to zero and cannot be seen in momentum space. However, one can evaluate the diagram in real space, and it is still absent. Fundamentally this is due to the fact that the conventional perturbation theory is perturbative in orders of the gauge field, which breaks down with uniform field strength. Nevertheless, combining the two calculation, we can still say that α_{3d} is a bulk property and is independent of the boundaries. α_{wzw}, on the other hand, is similar to the polarization: it does depend on the boundary, but when there is no boundary, it presents itself as a Berry's phase. Note that one benefit of using the Green's function is that the separation of the local terms and boundary terms matches exactly how the

expression depends on the extra dimension or not. This is not the case if we use the density matrices, either to calculate the same Berry's phase[30], or to calculate a current response to a pumping procedure[19]. In both calculations the ME tensor naturally separates into two terms, with the first term independent of the energy gap:

$$\alpha = \alpha_{\rm cs} + \alpha_{\rm G}; \tag{6.4}$$

$\alpha_{\rm cs}$ is isotropic, but $\alpha_{\rm G}$ is not traceless. While $\alpha_{\rm G}$ can be uniquely determined by the bulk band structure and is independent of the boundaries, its trace is actually not measurable in the bulk.

Let us now focus at the isotropic part $\alpha_{\rm wzw}$. In terms of polarization in a magnetic field, the ambiguity is no surprise. However, how does the ambiguity of the orbital magnetization in a electric field come about?

One origin of the ambiguity is from the fact that the perturbation of a uniform electric field grows with distance. It therefore naturally depends on the boundary, when there is one. When we consider periodic boundary conditions, however, it becomes less clear.

In order to study the OES with periodic boundary conditions, we first have to properly define the magnetization with periodic boundary conditions. Without the current at the boundary, one sensible definition of the magnetization is from the relation $B = H + M$. That is, in the absence of applied current (which generates H), the magnetization simply equals the measured magnetic field. Note that with periodic boundary conditions and a finite volume, the magnetic field is quantized, because the total magnetic flux through the sample is quantized in units of h/e. In this case we take the perspective that the magnetic field will take the closest quantized value to the magnetization while the magnetization itself is still continuous.

In our previous work[30], we have shown that in a magnetic field, the θ term, which characterizes the isotropic part of the OMP, changes the quantization condition of the global electric flux. The ground state of the system thus carries an electric flux of -$(\theta e^2/2\pi h)\Phi_B +$ ne, where n is some integer that minimizes the flux. Using $0 = D = E + P$, the θ term thus gives an isotropic orbital magneto-polarization response $\frac{\partial P}{\partial B} = \frac{\theta e^2}{2\pi h}$. However, this result is valid only when $(\Phi_B \theta e/2\pi h) < 1$. In the thermodynamic limit this condition is always violated, and instead $\frac{\partial P}{\partial B} = 0$.

Similarly, to see whether the same term contributes to the OES of the system, we would like to investigate whether there is a uniform magnetic field, when we constrain the path integral to have a given average electric field in the same direction. However, the electric field and the magnetic field behave in intrinsically different ways, when we formulated our theory assuming the existence of electric charges and the absence of magnetic monopoles: the quantization of the electric flux can change in the presence of the magnetic field, while the quantization of the magnetic flux is fixed at (h/e). When we apply an electric flux, we can always imagine that the system is a coherent state composed of states with integer electric fluxes. The background magnetic field therefore does not have to be different from zero. Therefore, even at finite size, the θ term does not give rise to the OES. *The Maxwell relation between the the isotropic OMP and the OES are thus violated.* They are only equal in the thermodynamic limit, where the θ term gives no contribution for both quantities. In other words, the isotropic OES is better thought of as a bulk-induced surface response, which vanishes when there is no boundary surfaces.

Now let us consider geometry with boundaries in some detail. From the result of Ref. [39], we know that with open boundary conditions in all directions, the OES has an ambiguity only determined by specific surface boundary conditions. We have also seen in the introduction that in a cylinder geometry, the ambiguity of the OES can come from the quantized Hall current on the side surfaces.

What if there are no side surfaces? Suppose we take periodic boundary conditions only in two directions to get rid of the side surfaces. Does the OES still have the same ambiguity? One naively would expect the situation to be similar to the case with periodic boundary conditions, due to the absence of the possible circulating Hall currents. However, a more careful argument shows it is not the case. In fact, the system will spontaneously generate a magnetic field, which will then generate surface charge density $\sigma = \pm(\nu + \theta/2\pi)e^2B/h$ via the OMP response, to lower the electric energy. Minimizing the total energy as a function of B, we then get $B = M = (\nu + \theta/2\pi)e^2E/h$. While at finite size the total magnetic flux is quantized in units of h/e in this setup, in the thermodynamic limit, the magnetic field will converge to the expected value, in contrast to the situations with periodic boundary conditions where it stays at zero. We have numerically confirmed this result by calculating the magnetization in the electric field, using the momentum space formula for the magnetization, derived in Ref. [37], as shown in Fig. 6-3.

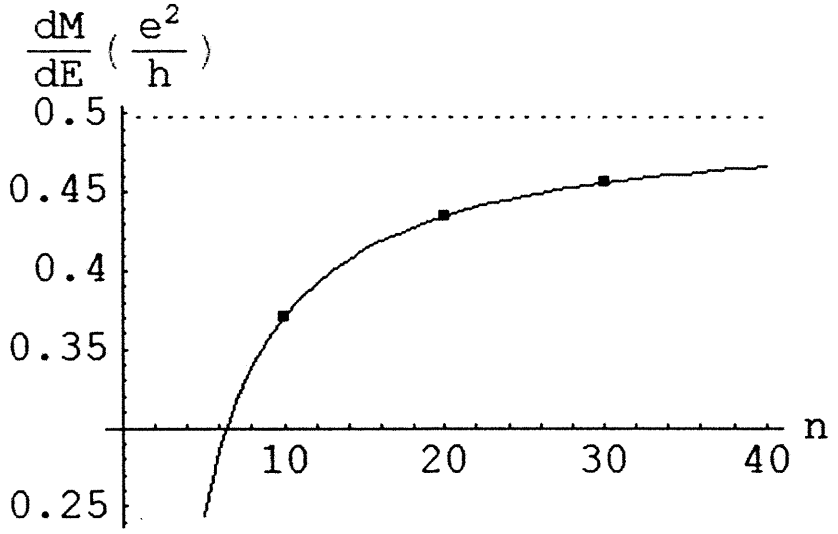


Figure 6-3: Here we plot the calculated OES versus the number of layers in the z-direction, with the model described by Eq. (73) in Ref. [16] with $\theta = 0$, $m = c = 1$. We take $\theta = 0.5\pi$ at the top and the bottom layer to gap out the edge states. (If we take $\theta = \pm 0.5\pi$ on the two surfaces respectively, the whole system will be a Chern insulator and can no long be kept at charge neutrality without closing the gap in a magnetic field.) We put on an electric field such that the potential difference between the top and the bottom layer is 0.2. The boxes show the calculated values. The solid curve is a fit by assuming a fixed width w of the surface charges when there is a magnetic field, such that $\frac{\mathrm{d}M}{\mathrm{d}E} \propto (1 - \frac{w}{n})$. The fit gives gives $\frac{\mathrm{d}M}{\mathrm{d}E} = 0.50\frac{e^2}{h}$ in the thermodynamic limit and $w = 2.54$. The OES changes sign as expected, when we change to $\theta = -0.5\pi$ instead on the boundary.

Before summing up, let us consider how gapless surface states can alter the ME response. Evidently, if we attach a fractional quantum Hall state on the side of the cylinder, the OES is going to change by a fraction of e^2/h.[47] In general the fraction is quite arbitrary, so in this case the bulk value of the isotropic OES is not valid. This corresponds to the fact that the fractional quantum Hall state has ground state degeneracy. In general, we will therefore expect any gapless surface state will destroy the bulk description of the isotropic ME response.

To sum up, The anisotropic part of the ME tensor $\alpha_{3\mathrm{d}}$ is independent of the boundaries. The isotropic part α_{wzw} depends partially on the boundary. While $\alpha_{3\mathrm{d}}$ is a truly local quantity, α_{wzw} only lives at $q = 0$. Corroborating with the fact that both isotropic OES and OMP responses vanish with periodic boundary conditions in the thermodynamic limit, it is better to think of α_{wzw} as a quantized surface effect induced by the bulk.

6.4 Conclusion

We have thus gone through polarization, magnetization, and magneto-electric responses and see their dependence on the boundary. A bulk calculation done with periodic boundary conditions contains enough information to predict how the quantity in question can depend on the boundary, however. In particular, using our formalism described in Ref. [46], any quantity that does not involve an extension of the Green's function to one extra dimension, such as the magnetization in zero electric field, is independent of the boundary. On the other hand, quantities that requires an extension to extra dimension, such as the polarization and the isotropic magneto-electric effect, will depend on the boundary. The bulk can determine its value up to some quantized amount, only when (i) there are no gapless surface states, (ii) surfaces break no symmetry that is required to determine the bulk value with periodic boundary conditions, and (iii) the system is kept at charge neutrality. If any of the conditions are violated, the surface contribution will dominate and render the results obtained with periodic boundary conditions invalid. For thermodynamic quantities of this kind, they cannot be measured in the bulk, without careful control at the boundary. Specifically, one cannot do a local measurement to distinguish the topological insulator in 3d from a trivial insulator, because (i) the coefficient of the θ-term will depend on the boundary; (ii) it is absent at finite q.

Chapter 7

Conclusions and Outlook

In this thesis, we have thus far focused on insulators and their electromagnetic effective action. We have shown that the topological term will arises in odd spatial dimensions, with the coefficient given by the WZW-like combination of the Green's functions. In three spatial dimensions, however, there are other non-topological part of the response which together with the topological term gives the anisotropic magneto-electric response, when the time reversal symmetry is broken.

In addition to our original goal of understanding how the topological index appear in the effective theory, our formalism provides more. From the perspective of the formalism, it is only when the effective action requires a quantized coefficient that the topological index can be singled out. Generically, topological and non-topological responses can mix together, as illustrated by the example of the magneto-electric response.

On the other hand, the electric field and the magnetic field behave quite differently in the bulk. The orbital electric-susceptibility and the orbital magneto-polarizability only agree with each other when there is a boundary. We find that we can distinguish between bulk quantities by their dependence on the boundary.

Our formalism is not limited to insulators. One can also consider superconductors, where superfluid velocity plays an additional role. Recently there has been development on Weyl semimetals, and the formalism also seems to be an ideal fit.

Appendix A

Path Integral Formulation for the θ term in One Spatial Dimension

In the main text, we derive the physical consequence of the θ-term using the notion of θ-vacuum, which is similar to a Hamiltonian formalism. One may wonder why we do not directly carry out the path integral. The first reason is that the quantization is not obvious if we just do the euclidean path integral as done below. The second reason is that if we calculate the fluctuation of the electric field at finite temperature, a naive calculation would give us a sum of *negative* values, which does not make sense. It turns out that for a free theory the position space path integral is ill-behaved and a positive finite term is expanded as an infinite negative sum. A similar situation occurs when one calculates the ground state energy of the bosonic string using mode expansion. Let we start right from the Lagrangian

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{e\theta}{2\pi}\epsilon^{\mu\nu}\partial_\mu A_\nu \tag{A.1}$$

using the gauge $A_0 = 0$, for the $q = 0$ sector at finite temperature $1/\beta$ we have the partition function

$$Z'_{q=0} = \left(\prod_{\omega_i}\left(\frac{2\pi}{\beta L\omega_i^2}\right)\right)\sum_n e^{in\theta}\exp\left(-\frac{1}{2\beta L}(\frac{2\pi n}{e})^2\right), \tag{A.2}$$

where $\omega_i = 2\pi i/\beta$ are the Matsubara frequencies. Again the finite frequency part decouples and the zero frequency part agrees with Eq. 3.8 if we integrate ℓ first instead:

$$Z'_{q=0} \propto Z_{q=0} = \sum_n e^{in\theta}e^{-\frac{1}{2\beta L}(\frac{2\pi n}{e})^2} \equiv \sum_n W_n. \tag{A.3}$$

Nevertheless, it is hard to see from this form that θ corresponds to a quantization condition for the electric field. Without reversing the ℓ integral, another way to see the θ-dependence is to calculate the expectation value and the fluctuation of the electric field. For $\theta = \pi$, the expectation value would vanish and we can only rely on the fluctuation.

If we calculate $\langle|\tilde{E^1}(0)|^2\rangle$, however, we would encounter a problem in the path integral as now all finite frequency part contributes and their sum seems to be infinitely negative:

$$\langle|\tilde{E^1}(0)|^2\rangle = \frac{L^2}{Z_0}\left(\sum_n -\left(\frac{2\pi n}{\beta L e}\right)^2 W_n\right) - \sum_i \frac{2L}{\beta}. \tag{A.4}$$

If we compare this to what we would have got using the Hamiltonian formalism,

$$\langle|\tilde{E^1}(0)|^2\rangle = \frac{L^2}{Z_0}\left(\sum_n W_n\left(-\left(\frac{2\pi n}{\beta L e}\right)^2 + \frac{1}{\beta L}\right)\right). \tag{A.5}$$

It seems we have to require

$$\sum_i (\mathbf{1}) = -\frac{1}{2}. \tag{A.6}$$

for the two expressions to agree. We can understand this equality by thinking of the left hand side as the zeta function at zero, $\zeta(0)$, written in a series. While the series is divergent at zero, the zeta function is well-defined and is indeed $-\frac{1}{2}$.

The function $\sum_n n^2 W_n$ is related to the elliptic Θ-function. If one subtracts the fluctuation at $\theta = 0$ from the expression and calculate at $\beta \to \infty$, one recovers that

$$\langle|\tilde{E^1}(0)|^2\rangle - \langle|\tilde{E^1}(0)|^2\rangle|_{\theta=0} = L^2 e^2 \left(\frac{\theta}{2\pi}\right)^2, \tag{A.7}$$

which implies the quantization.

Appendix B

Topological Combination of Green's Functions

In this appendix, we first discuss what kind of combinations of Green's functions are topological, then we provide some formulas we have used in the main text.

When we say an integral is topological, we mean that the value of the integral is independent of any smooth deformations that leaves the integrand on the boundary unaltered. For example, the following integral is topological:

$$I = \int \mathrm{d}\omega \, \mathrm{tr}\big(g\partial_\omega g^{-1}\big) \tag{B.1}$$

$$\begin{aligned}
\delta I &= \int \mathrm{d}\omega \, \mathrm{tr}\big(\delta g \partial_\omega g^{-1} + g\partial_\omega \delta g^{-1}\big) \\
&= \int \mathrm{d}\omega \, \mathrm{tr}\big(\delta g \partial_\omega g^{-1} + \partial_\omega(g\delta g^{-1}) - \partial_\omega g \delta g^{-1}\big) \\
&= \int \mathrm{d}\omega \, \mathrm{tr}\big(\delta g \partial_\omega g^{-1} + \partial_\omega(g\delta g^{-1}) + \partial_\omega g g^{-1}\delta g g^{-1}\big) \\
&= \int \mathrm{d}\omega \, \mathrm{tr}\big(\partial_\omega(g\delta g^{-1})\big);
\end{aligned} \tag{B.2}$$

we have used $\delta(gg^{-1}) = \partial_\omega(gg^{-1}) = 0$ in the last two equailties. We see that the variation δI is a total derivative of a single-valued function, which implies that it is zero if the integrand is not varied on the boundary. Notice here we did not assume any particular form of g; that is, I is topological under arbitrary smooth deformation of g.

We can construct similar topologically-invariant integrals in higher dimensions. In fact,

$$I^{2d} = \int \mathrm{d}\omega \mathrm{d}^{2d}k\, \epsilon^{a_1 a_2 \ldots a_{2d+1}} \mathrm{tr}\Big(\prod_{i=1}^{2d+1} (g\partial_{a_i} g^{-1}) \Big) \tag{B.3}$$

is topological. To prove this, we notice first that when we have an even number of $(g\partial_{a_i} g^{-1})$ multiplied together with their indices antisymmetrized, they become a total derivative:

$$\begin{aligned} & \epsilon^{a_1 a_2 \ldots a_{2d}} \prod_{i=1}^{2d} (g\partial_{a_i} g^{-1}) \\ = \;& \epsilon^{a_1 a_2 \ldots a_{2d}} (-1)^d \prod_{j=1}^{d} (\partial_{a_{2j-1}} g)(\partial_{a_{2j}} g^{-1}) \\ = \;& \epsilon^{a_1 a_2 \ldots a_{2d}} (-1)^d \partial_{a_1} \big(g\partial_{a_2} g^{-1} \prod_{j=2}^{d} (\partial_{a_{2j-1}} g)(\partial_{a_{2j}} g^{-1}) \big). \end{aligned} \tag{B.4}$$

Now we consider a general deformation:

$$\begin{aligned} \delta I^{2d} &= (2d+1) \int \mathrm{d}\omega \mathrm{d}^{2d}k\, \epsilon^{a_1 a_2 \ldots a_{2d+1}} \mathrm{tr}\big(\delta(g\partial_{a_1} g^{-1}) \prod_{i=2}^{2d+1} (g\partial_{a_i} g^{-1}) \big) \\ &= (2d+1) \int \mathrm{d}\omega \mathrm{d}^{2d}k\, \epsilon^{a_1 a_2 \ldots a_{2d+1}} \mathrm{tr}\big((\delta g\partial_{a_1} g^{-1} + \partial_{a_1}(g\delta g^{-1}) + \partial_{a_1} g g^{-1} \delta g g^{-1}) \prod_{i=2}^{2d+1} (g\partial_{a_i} g^{-1}) \big) \\ &= (2d+1) \int \mathrm{d}\omega \mathrm{d}^{2d}k\, \epsilon^{a_1 a_2 \ldots a_{2d+1}} \mathrm{tr}\big((\delta g\partial_{a_1} g^{-1} - g\partial_{a_1} g^{-1} \delta g g^{-1}) \prod_{i=2}^{2d+1} (g\partial_{a_i} g^{-1}) \\ &\quad + \partial_{a_1}(g\delta g^{-1} \prod_{i=2}^{2d+1} (g\partial_{a_i} g^{-1})) \big) \\ &= (2d+1) \int \mathrm{d}\omega \mathrm{d}^{2d}k\, \epsilon^{a_1 a_2 \ldots a_{2d+1}} \mathrm{tr}\big(\partial_{a_1}(g\delta g^{-1} \prod_{i=2}^{2d+1} (g\partial_{a_i} g^{-1})) \big); \end{aligned} \tag{B.5}$$

the second-to-last equality follows from the fact that the product term is already a total derivative and with antisymmetricity of the indices, the product of two total derivatives result in another total derivative. The last equality comes from the cyclic property of the trace and the first two terms cancel each other. We therefore have showed that I_{2d} is topological for any d. Notice that even when g satisfies a twisted boundary condition $g(k+G) = U^\dagger g(k) U$ on a closed manifold, the variation still vanishes.

In the discussion we have in the main text, however, we have concentrated on non-interacting systems, where the Green's function is taken to be in the form of $(\omega - H_k \pm i\delta)^{-1}$.

We thus are more interested in integrals of Green's functions that are topological subject only to any smooth deformation of H_k, instead of an arbitrary deformation of g. Fortunately, since $\partial_\omega g^{-1} = 1$ with the non-interacting Green's function, we can directly translate the topological combination above to combinations that is invariant under only the deformation of H_k. The invariant reads

$$I_F^{2d} = \int \mathrm{d}\omega \mathrm{d}^{2d}k \, \epsilon^{a_1 a_2 \ldots a_{2d}} \mathrm{tr}\big((\prod_{i=1}^{2d}(g\partial_{a_i} g^{-1}))g\big). \tag{B.6}$$

The indices now only run through all the spatial directions.

Next we show the derivation of Eq. (5.19). Since the Berry's phase is invariant under small deformations of the Green's function extended into the surface, the integral has to be topological. By dimensional counting we immediately see that I_F^2 is a possible candidate. The rest of the task is to find the constant in front, as well as any possible total derivatives.

$$\begin{aligned}
& \frac{1}{2}\int_S \mathrm{d}^2k\epsilon^{ij}\mathrm{Tr}\left(g\partial_i g^{-1}\partial_j g\right) \\
= \; & \frac{1}{2}\int_S \mathrm{d}^2k \int \frac{\mathrm{d}\omega}{2\pi}\epsilon^{ij}\mathrm{tr}\left(g\partial_i g^{-1}\partial_j g\right) \\
= \; & \frac{1}{2}\int_S \mathrm{d}^2k \int \frac{\mathrm{d}\omega}{2\pi}\epsilon^{ij}\sum_{mn}\frac{\langle u_m|\partial_i H_k|u_n\rangle\ \langle\partial_j u_n|u_m\rangle}{(\omega-E_m)(\omega-E_n)} \\
= \; & \frac{1}{2}\int_S \mathrm{d}^2k \int \frac{\mathrm{d}\omega}{2\pi}\epsilon^{ij}\sum_{mn}\frac{(E_n-E_m)\langle u_m|\partial_i u_n\rangle\langle\partial_j u_n|u_m\rangle}{(\omega-E_m)(\omega-E_n)} \\
= \; & \int_S \mathrm{d}^2k\epsilon^{ij}\sum_{m\in\mathrm{emp},n\in\mathrm{occ}} i\langle\partial_i u_n|u_m\rangle\langle u_m|\partial_j u_n\rangle \\
= \; & \int_S \mathrm{d}^2k\epsilon^{ij}\sum_{n\in\mathrm{occ}} i\langle\partial_i u_n|\partial_j u_n\rangle \\
= \; & \oint_{\partial S}\mathrm{d}k^\ell\sum_{n\in\mathrm{occ}} i\langle u_n|\partial_\ell u_n\rangle.
\end{aligned} \tag{B.7}$$

As we can see, there are no extra total derivative terms. If we integrate this term on a torus, as we did in Eq. (5.21), we get

$$\begin{aligned}
\frac{1}{2}\int_{\mathrm{BZ}}\mathrm{d}^2k\epsilon^{ij}\mathrm{Tr}\left(g\partial_i g^{-1}\partial_j g\right) &= \int_{BZ}\mathrm{d}^2k\epsilon^{ij}\sum_{n\in\mathrm{occ}} i\langle\partial_i u_n|\partial_j u_n\rangle \\
&= 2\pi C_1.
\end{aligned} \tag{B.8}$$

Similarly, we can relate I_F^4 to C_2, the second Chern number if integrated on a four

dimensional manifold without boundaries. In Ref.[16], they use dispersionless bands to derive the ratio betwenn I_F^4 and C_2. Here we just quote their result (with an extra factor of $(-i)$ since they are using the imaginary time Green's function):

$$\begin{aligned} C_2 &\equiv \frac{1}{32\pi^2}\int \mathrm{d}^4k\epsilon^{ijk\ell}\mathrm{tr}\big(\mathcal{F}_{ij}\mathcal{F}_{k\ell}\big) \\ &= \frac{i}{48\pi^2}I_F^4, \end{aligned} \tag{B.9}$$

with

$$\mathcal{F}_{ij}^{nn'} = \partial_i\mathcal{A}_j^{nn'} - \partial_j\mathcal{A}_i^{nn'} + i[a_i, a_j]^{nn'} \tag{B.10}$$

is the Berry's phase gauge field strength. Rather remarkably, the two integral no longer agree with each other when integrated on a manifold with a boundary. In this case, they differ by a globally defined total derivative.

Appendix C

From the Green's Function Expression of the OMP to Expression in Energy Eigenbasis

Before we start to evaluate equation (5.48), we emphasize again that our distinction between α_{topo} and α_{exact} is different from the distinction between α_{CS} and α_{G} in Ref.[19]. Specifically, α_{exact} is traceless, as can be seen from Eq. (5.41), whereas α_G in general is not. With this in mind, let us start from α_{exact}:

$$\alpha_{3\text{d}ij} = -\frac{i}{6}\epsilon_{abj}\big((iab) - c.c.\big). \tag{C.1}$$

As done in the main text, we use (iab) in short for $\text{Tr}(g\partial_i g^{-1} g\partial_a g^{-1} g\partial_b g^{-1} g)$. The capital trace again denotes tracing over all the bands and integrating over all the momentum and energy divided by (2π) for each direction. Expanding in the energy eigenbasis, we get

$$\begin{aligned}
(iab) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\mathrm{d}\omega}{2\pi}\sum_{n,\ell,m}\frac{\langle m\,|\partial_i H|\,n\rangle\ \langle n\,|\partial_a H|\,\ell\rangle\ \langle \ell\,|\partial_b H|\,m\rangle}{(\omega - E_m)^2(\omega - E_n)(\omega - E_\ell)} \\
&= i\int \frac{\mathrm{d}^3k}{(2\pi)^3}\Bigg(- \text{sgn}(E_n)\theta(-E_nE_\ell)\theta(-E_nE_m)\frac{1}{E_n - E_m}\langle\partial_i m|n\rangle\langle\partial_a n|\ell\rangle\ \langle\ell\,|\partial_b H|\,m\rangle \\
&- \text{sgn}(E_\ell)\theta(-E_\ell E_m)\theta(-E_\ell E_n)\frac{1}{E_\ell - E_m}\ \langle m\,|\partial_i H|\,n\rangle\ \ \langle\partial_a n|\ell\rangle\langle\partial_b \ell|m\rangle \\
&- \text{sgn}(E_m)\theta(-E_nE_m)\theta(-E_\ell E_m)\frac{1}{E_n - E_m}\langle\partial_i m|n\rangle\ \langle n\,|\partial_a H|\,\ell\rangle\ \ \langle\partial_b \ell|m\rangle
\end{aligned}$$

$$
\begin{aligned}
&- \operatorname{sgn}(E_m)\theta(-E_nE_m)\theta(-E_\ell E_m)\frac{1}{E_\ell - E_m}\langle\partial_i m|n\rangle\,\langle n\,|\partial_a H|\,\ell\rangle\;\langle\partial_b \ell|m\rangle\Big) \\
&= i\int\frac{\mathrm{d}^3k}{(2\pi)^3}\sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\Big(\frac{1}{E_n - E_m}\langle\partial_i m|n\rangle\langle\partial_a n|m'\rangle\,\langle m'\,|\partial_b H|\,m\rangle \\
&+ \frac{1}{E_{n'} - E_m}\langle m\,|\partial_i H|\,m'\rangle\;\langle\partial_a m'|n'\rangle\langle\partial_b n'|m\rangle - \frac{1}{E_{n'} - E_m}\langle\partial_i m|n\rangle\,\langle n\,|\partial_a H|\,n'\rangle\;\langle\partial_b n'|m\rangle \\
&- \frac{1}{E_n - E_m}\langle\partial_i m|n\rangle\,\langle n\,|\partial_a H|\,n'\rangle\;\langle\partial_b n'|m\rangle\Big) - (\mathrm{occ}\leftrightarrow\mathrm{emp}); \qquad \text{(C.2)}
\end{aligned}
$$

we have used $|n\rangle$ to denote $|u_{nk}\rangle$ to avoid cluttering the expression.

Since α_{wzw} is isotropic, the off-diagonal tensor element comes entirely from $\alpha_{3\mathrm{d}}$. Without loss of generality, let us look at α_{yz}:

$$
\begin{aligned}
\alpha_{yz} &= -\frac{i}{6}\epsilon^{abz}\big((yab) - c.c.\big) \\
&= -\frac{i}{6}\Big(\big((yxy) - (yyx)\big) - c.c.\Big). \qquad \text{(C.3)}
\end{aligned}
$$

In the last equality of Eq. (C.2), the first and the last term are already in the form as derived in Ref. [19]. Let us look at the two terms in the middle as we first plug in $i = y$, $a = x$, $b = y$:

$$
\begin{aligned}
&\sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\Big(\frac{1}{E_{n'} - E_m}\,\langle m\,|\partial_y H|\,m'\rangle\;\langle\partial_x m'|n'\rangle\langle\partial_y n'|m\rangle - (\mathrm{occ}\leftrightarrow\mathrm{emp})\Big) \\
&= \sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\Big(\frac{1}{E_{n'} - E_m}\langle\partial_y n'|m\rangle\,\langle m\,|\partial_y H|\,m'\rangle\;\langle\partial_x m'|n'\rangle \\
&+ \frac{1}{E_n - E_m}\langle\partial_y m|n\rangle\,\langle n\,|\partial_y H|\,n'\rangle\;\langle\partial_x n'|m\rangle\Big); \qquad \text{(C.4)}
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\Big(\frac{-1}{E_{n'} - E_m}\langle\partial_y m|n\rangle\,\langle n\,|\partial_x H|\,n'\rangle\;\langle\partial_y n'|m\rangle - (\mathrm{occ}\leftrightarrow\mathrm{emp})\Big) \\
&= \sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\Big(-\frac{1}{E_{n'} - E_m}\langle\partial_y n'|m\rangle\langle\partial_y m|n\rangle\,\langle n\,|\partial_x H|\,n'\rangle \\
&- \frac{1}{E_{n'} - E_m}\langle\partial_y m|n'\rangle\langle\partial_y n'|m'\rangle\,\langle m'\,|\partial_x H|\,m\rangle\;\Big). \qquad \text{(C.5)}
\end{aligned}
$$

Similarly, when we plug in $i = y$, $a = y$, $b = x$ and sum with its complex conjugate, we find

that every term cancels out:

$$\sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\Bigg(\quad \frac{1}{E_{n'}-E_m}\langle m\,|\partial_y H|\,m'\rangle\ \langle\partial_y m'|n'\rangle\langle\partial_x n'|m\rangle$$
$$-\ \frac{1}{E_{n'}-E_m}\langle\partial_y m|n\rangle\,\langle n\,|\partial_y H|\,n'\rangle\ \langle\partial_x n'|m\rangle-(\mathrm{occ}\leftrightarrow\mathrm{emp})\Bigg)+c.c.=0. \tag{C.6}$$

Summing over, we then have

$$\Big(\quad(\quad(yxy)-(yyx))-c.c.\Big)$$
$$=\ 3i\int\frac{\mathrm{d}^3k}{(2\pi)^3}\sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\left(\frac{\epsilon^{ab}}{E_n-E_m}\langle\partial_y m|n\rangle\langle\partial_a n|m'\rangle\,\langle m'\,|\partial_b H|\,m\rangle\ -(\mathrm{occ}\leftrightarrow\mathrm{emp})\right)$$
$$-\ c.c.; \tag{C.7}$$

here a and b run through only x and y. We finally have

$$\alpha_{yz}\ =\ \frac{1}{2}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\sum_{m,m'\in\mathrm{emp};n,n'\in\mathrm{occ}}\left(\frac{\epsilon^{ab}}{E_n-E_m}\langle\partial_y m|n\rangle\langle\partial_a n|m'\rangle\,\langle m'\,|\partial_b H|\,m\rangle\ -(\mathrm{occ}\leftrightarrow\mathrm{emp})\right)$$
$$+\ c.c., \tag{C.8}$$

which is identical to the expression in Ref. [19].

As for the diagonal components, we have to expand the isotropic term α_{wzw}. The calculation is similar to Eq. (C.2), except that we have to rearrange terms into total derivatives and then integrate back to the physical momentum space. We currently are not aware of any special trick to automatically rearrange the terms into total derivatives other than the $\mathcal{F}\wedge\mathcal{F}$ part, which corresponds to α_{CS} in Ref. [19]; nevertheless, we can use the Stokes theorem to convert the difference between α_G in Ref. [19] and $\alpha_{3\mathrm{d}}$ to the extended space and verify that it agrees with the remaining parts in α_{wzw}:

$$\begin{aligned}&(\alpha_G-\alpha_{3\mathrm{d}})_{ij}\\ =\ &-\frac{1}{6}\delta_{ij}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\epsilon^{abc}\,\langle m\,|\partial_a H|\,m'\rangle\ \langle\partial_b m'|n\rangle\frac{\langle\partial_c n|m\rangle}{E_n-E_m}+c.c.\\ &-(\mathrm{occ}\leftrightarrow\mathrm{emp})\\ =\ &-\frac{\pi}{3}\delta_{ij}\int\frac{\mathrm{d}^4k}{(2\pi)^4}\epsilon^{abcd}\partial_a\Big(\,\langle m\,|\partial_b H|\,m'\rangle\ \langle\partial_c m'|n\rangle\frac{\langle\partial_d n|m\rangle}{E_n-E_m}\Big)\end{aligned}$$

$$+c.c. - (\text{occ} \leftrightarrow \text{emp}). \tag{C.9}$$

We now start to expand α_{wzw}:

$$\begin{aligned}
\epsilon^{abcd} \quad & \mathrm{Tr}^S(\mathbf{g}\partial_a\mathbf{g}^{-1}\mathbf{g}\partial_b\mathbf{g}^{-1}\mathbf{g}\partial_c\mathbf{g}^{-1}\mathbf{g}\partial_d\mathbf{g}^{-1}\mathbf{g}) \\
= & \int_S \frac{\mathrm{d}^4k}{(2\pi)^4}\int\frac{\mathrm{d}\omega}{2\pi}\sum_{ijkl}\epsilon^{abcd}\frac{\langle i\,|\partial_a H|\,j\rangle\ \langle j\,|\partial_b H|\,k\rangle\ \langle k\,|\partial_c H|\,\ell\rangle\ \langle \ell\,|\partial_d H|\,i\rangle}{(\omega-E_i)^2(\omega-E_j)(\omega-E_k)(\omega-E_\ell)} \\
\equiv & \int_S \frac{\mathrm{d}^4k}{(2\pi)^4}\big(J_{(ik,j\ell)} + (J_{(ij,k\ell)} - c.c.) + J_{(i,jk\ell)} + J_{(k,ij\ell)} + (J_{(j,ik\ell)} - c.c.)\big) - (\text{occ} \leftrightarrow \text{emp}).
\end{aligned} \tag{C.10}$$

We separate the contributions by different pole placements. $(ik, j\ell)$ for example implies that E_i and E_j are of the same sign and are opposite to E_k and E_ℓ. Here we illustrate the calculation by explicitly computing the contribution $J_{(ij,k\ell)}$; the calculation for the other contributions are similar and we shall just list the answer. To avoid cluttering the expression we use i to denote E_i as well when there is no ambiguity.

$$\begin{aligned}
-iJ_{(ik,j\ell)} &= \sum_{(ij,kl)} \mathrm{sgn}(j)\left(\frac{(i-j)(j-k)(k-\ell)(\ell-i)}{(j-i)^2(j-k)(j-\ell)} + \frac{(i-j)(j-k)(k-\ell)(\ell-i)}{(\ell-i)^2(\ell-j)(\ell-k)}\right)\times \\
&\quad \epsilon^{abcd}\langle\partial_a i|j\rangle\langle\partial_b j|k\rangle\langle\partial_c k|\ell\rangle\langle\partial_d \ell|i\rangle \\
&= \sum_{(ij,kl)} -\mathrm{sgn}(j)\left(\frac{(k-\ell)(\ell-i)}{(j-i)(j-\ell)} + \frac{(i-j)(j-k)}{(\ell-i)(\ell-j)}\right)\epsilon^{abcd}\langle\partial_a i|j\rangle\langle\partial_b j|k\rangle\langle\partial_c k|\ell\rangle\langle\partial_d \ell|i\rangle \\
&= \sum_{(ij,kl)} \mathrm{sgn}(j)\left(\frac{k-\ell}{j-i} - \frac{k-\ell}{j-\ell} + (j\leftrightarrow\ell)\right)\epsilon^{abcd}\langle\partial_a i|j\rangle\langle\partial_b j|k\rangle\langle\partial_c k|\ell\rangle\langle\partial_d \ell|i\rangle \\
&= \sum_{(ij,kl)} \mathrm{sgn}(j)\left(\frac{k-\ell}{j-i} - \frac{1}{2}\right)\epsilon^{abcd}\langle\partial_a i|j\rangle\langle\partial_b j|k\rangle\langle\partial_c k|\ell\rangle\langle\partial_d \ell|i\rangle + c.c. \\
&= \sum_{(ij,kl)} \mathrm{sgn}(j)\left(\frac{k-\ell+j-i}{j-i} - \frac{3}{2}\right)\epsilon^{abcd}\langle\partial_a i|j\rangle\langle\partial_b j|k\rangle\langle\partial_c k|\ell\rangle\langle\partial_d \ell|i\rangle + c.c. \\
&= \sum_{(ij,kl)} \mathrm{sgn}(j)\left(\frac{k-i}{j-i} + \frac{j-\ell}{j-i} - \frac{3}{2}\right)\epsilon^{abcd}\langle\partial_a i|j\rangle\langle\partial_b j|k\rangle\langle\partial_c k|\ell\rangle\langle\partial_d \ell|i\rangle + c.c. \\
&= \sum_{m,m'\in\text{emp},n,n'\in\text{occ}} \left(2\left(\frac{E_{n'}-E_n}{E_m-E_n}\right) - \frac{3}{2}\right)\epsilon^{abcd}\langle\partial_a n|m\rangle\langle\partial_b m|n'\rangle\langle\partial_c n'|m'\rangle\langle\partial_d m'|n\rangle + c.c. \\
&\quad - (\text{occ} \leftrightarrow \text{emp}).
\end{aligned} \tag{C.11}$$

To get to the first line, we have used

$$\langle i\,|\partial_a H|\,j\rangle \;= \partial_a E_i \delta_{ij} + (E_i - E_j)\langle \partial_a i|j\rangle. \tag{C.12}$$

In $J_{(ik,j\ell)}$ the first term on the right-hand-side does not contribute. In other parts however that term is important. In the fourth equality, we have taken advantage of the fact that exchanging j and ℓ gives the complex conjugate of the whole expression. We symmetrize the second fraction in the third equality with its complex conjugate to get $\frac{1}{2}$. In the second-to-last equality, the two fractions become each other with a negative sign when we exchange the occupied and empty states, therefore reaching the last equality.

The other contributions are given in the following:

$$\begin{aligned}
-i(J_{(ij,k\ell)} - c.c.) \;=\; & \sum_{n,n'\in \mathrm{occ}, m,m'\in \mathrm{emp}} 2\left(\frac{E_m - E'_m}{E_n - E_m} + \frac{E'_m - E_m}{E_n - E'_m}\right)\epsilon^{abcd} \times \\
& \langle \partial_a n|n'\rangle\langle \partial_b n'|m\rangle\langle \partial_c m|m'\rangle\langle \partial_d m'|n\rangle + c.c. \\
& + \sum_{n\in \mathrm{occ}; m,m'\in \mathrm{emp}} 2\left(\frac{(E_{m'} - E_m)\partial_a E_n}{(E_m - E_n)^2}\right)\epsilon^{abcd}\langle \partial_b m|m'\rangle\langle \partial_c m'|n\rangle\langle \partial_d n|m\rangle + c.c. \\
& - (\mathrm{occ} \leftrightarrow \mathrm{emp}); \qquad (C.13) \\
-iJ_{(k,ij\ell)} \;=\; & \sum_{n,n',n''\in \mathrm{occ}; m\in \mathrm{emp}} \left(\frac{(E_n - E_{n'})(E_n - E_{n''})}{(E_n - E_m)^2}\right)\epsilon^{abcd}\langle \partial_a n|n'\rangle\langle \partial_b n'|m\rangle\langle \partial_c m|m'\rangle\langle \partial_d m'|n\rangle \\
& + \sum_{n\in \mathrm{occ}; m,m'\in \mathrm{emp}} \left(\frac{(E_{m'} - E_m)\partial_a E_m}{(E_m - E_n)^2}\right)\epsilon^{abcd}\langle \partial_b m|m'\rangle\langle \partial_c m'|n\rangle\langle \partial_d n|m\rangle + c.c. \\
& - (\mathrm{occ} \leftrightarrow \mathrm{emp}); \qquad (C.14) \\
-iJ_{(i,jk\ell)} \;=\; & \sum_{n,n',n''\in \mathrm{occ}; m\in \mathrm{emp}} -\left(\frac{(E_n - E_{n'})(E_n - E_{n''})}{(E_n - E_m)^2}\right)\epsilon^{abcd}\langle \partial_a n|n'\rangle\langle \partial_b n'|m\rangle\langle \partial_c m|m'\rangle\langle \partial_d m'|n\rangle \\
& + \sum_{n,n',n''\in \mathrm{occ}, m\in \mathrm{emp}} \left(\frac{E_{n'} - E_{n''}}{E_m - E_n} - \frac{E_{n'} - E_{n''}}{E_m - E_{n'}}\right) \\
& \epsilon^{abcd}\langle \partial_a m|n\rangle\langle \partial_b n|n'\rangle\langle \partial_c n'|n''\rangle\langle \partial_d n''|m\rangle + c.c. \\
& - \sum_{n\in \mathrm{occ}; m,m'\in \mathrm{emp}} 2\left(\frac{(E_{m'} - E_m)\partial_a E_m}{(E_m - E_n)^2}\right)\epsilon^{abcd}\langle \partial_b m|m'\rangle\langle \partial_c m'|n\rangle\langle \partial_d n|m\rangle + c.c. \\
& + \sum_{n\in \mathrm{occ}; m,m'\in \mathrm{emp}} \left(\frac{\partial_a(E_{m'} - E_m)}{E_m - E_n}\right)\epsilon^{abcd}\langle \partial_b m|m'\rangle\langle \partial_c m'|n\rangle\langle \partial_d n|m\rangle + c.c. \\
& - (\mathrm{occ} \leftrightarrow \mathrm{emp}); \qquad (C.15) \\
-i(J_{(j,ik\ell)} - c.c.) \;=\; & \sum_{n,n',n''\in \mathrm{occ}, m\in \mathrm{emp}} \left(\frac{E_{n'} - E_{n''}}{E_m - E_n} - \frac{E_{n'} - E_{n''}}{E_m - E_{n'}}\right) \\
& \epsilon^{abcd}\langle \partial_a m|n\rangle\langle \partial_b n|n'\rangle\langle \partial_c n'|n''\rangle\langle \partial_d n''|m\rangle + c.c.
\end{aligned}$$

$$
\begin{aligned}
&+ \sum_{n\in\text{occ};m,m'\in\text{emp}} \left(\frac{\partial_a(E_{m'}-E_m)}{E_m-E_n}\right)\epsilon^{abcd}\langle\partial_b m|m'\rangle\langle\partial_c m'|n\rangle\langle\partial_d n|m\rangle + c.c. \\
&- \sum_{n\in\text{occ};m,m'\in\text{emp}} \left(\frac{(E_{m'}-E_m)\partial_a E_m}{(E_m-E_n)^2}\right)\epsilon^{abcd}\langle\partial_b m|m'\rangle\langle\partial_c m'|n\rangle\langle\partial_d n|m\rangle + c.c. \\
&- (\text{occ}\leftrightarrow\text{emp});
\end{aligned}
\tag{C.16}
$$

notice that every term (that is not canceled) come with its complex conjugate. The term in $J_{(ik,j\ell)}$ without energy dependence is the $\mathcal{F}\wedge\mathcal{F}$ term since

$$
\mathcal{F}_{ab}^{nn'} = \sum_{m\in emp} -i\langle\partial_a n|m\rangle\langle\partial_b m|n'\rangle - (a\leftrightarrow b). \tag{C.17}
$$

The remaining terms sum up to be the following total derivative, as one can verify by taking the derivative on every term in the bracket in the following:

$$
-iJ_{\text{tot}} = 2\epsilon^{abcd}\partial_a\left(\langle m\,|\partial_b H|\,m'\rangle\ \langle\partial_c m'|n\rangle\frac{\langle\partial_d n|m\rangle}{E_n-E_m}\right). \tag{C.18}
$$

By comparing this expression to Eq. (C.9), we finally recover Eq. (5.48).

Appendix D

Deriving the Orbital Magneto-Polarizability Using the Density Matrix Perturbation Theory

Similar to the use of Green's functions as discussed in Sec. 5.3, we can express the integral as a whole in terms of the density matrix by the following trick. The accumulated Berry's phase can be expressed as an integral of the Berry's curvature in one extra dimension using Stokes theorem, with the region of integration bounds by the original k_z integral. The Berry's curvature can now readily be expressed in terms of the density matrix extended into the extra dimension, which is chosen continuously but otherwise aribitrarily with the constraint such that on the boundary, we have the original density matrix. We therefore have

$$\begin{aligned} i\oint_{\partial S} \mathrm{dk_z}\langle\Psi_{\tilde{\mathrm{B}}}|\frac{\partial}{\partial \mathrm{k_z}}|\Psi_{\tilde{\mathrm{B}}}\rangle &= i\int_S \mathrm{d^2k}\epsilon^{\alpha\beta}\partial_\alpha\langle\tilde{\Psi}_{\tilde{\mathrm{B}}}|\partial_\beta|\tilde{\Psi}_{\tilde{\mathrm{B}}}\rangle \\ &= i\int_S \mathrm{d^2k}\epsilon^{\alpha\beta}\mathrm{Tr}\left(\tilde{\rho}\partial_\alpha\tilde{\rho}\partial_\beta\tilde{\rho}\right); \end{aligned} \tag{D.1}$$

$|\tilde{\Psi}_{\vec{B}}\rangle$ is the 2D electron many-body wave function, which in addition to being a function of k_z, has been extended to some extra direction k_w. $\tilde{\rho} = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|$ is the extended 2D

single particle density matrix, where $|\tilde{\psi}_i\rangle$ is a 2D single particle eigenstate in magnetic field $\vec{B}$. α, β run through two directions which is spanned by k_z and k_w. The trace sums over both the band and the (x, y)-position basis. As mentioned above, the integral is chosen to be performed on the area such that the boundary is at $(k_z, k_w = 0)$ and the density matrix has known values. The second equality comes from the following calculation: first we note $|\Psi_B\rangle = \det(\psi_i)$, and

$$\partial_\alpha \langle \Psi_B | \partial_\beta | \Psi_B \rangle = \sum_i \partial_\alpha \langle \psi_i | \partial_\beta | \psi_i \rangle. \tag{D.2}$$

Now we plug in $\rho = \sum_i |\psi_i\rangle\langle\psi_i|$ to the right hand side of the second equality, we have

$$\begin{aligned} \mathrm{Tr} \quad & (\rho \partial_\alpha \rho \partial_\beta \rho) \\ = \quad & \sum_{ijk} |\psi_i\rangle\langle\psi_i| \Big((\partial_\alpha |\psi_i\rangle)\langle\psi_i| + |\psi_i\rangle(\partial_\alpha \langle\psi_i|) \Big) \\ & \Big((\partial_\beta |\psi_i\rangle)\langle\psi_i| + |\psi_i\rangle(\partial_\beta \langle\psi_i|) \Big) \\ = \quad & \sum_{ij} \langle\psi_i|\partial_\alpha|\psi_j\rangle\langle\psi_j|\partial_\beta|\psi_i\rangle \\ & + \sum_i (\partial_\alpha \langle\psi_i|)(\partial_\beta|\psi_i\rangle); \end{aligned} \tag{D.3}$$

in the derivation we have taken advantage of the fact that $\langle\psi_i|\psi_j\rangle = \delta_{ij}$ and thus $(\partial_\alpha\langle\psi_i|)|\psi_j\rangle = -\langle\psi_i|\partial_\alpha|\psi_j\rangle$. Contract both Eq. D.2 and Eq. D.3 with $\epsilon^{\alpha\beta}$, we can see that they agree.

Different choices of density matrices inside the boundary can only alter the integral by multiples of $2\pi i$. To avoid cluttering of the equations, in the following we omit the tilde for the extended objects when there is no ambiguity.

Then following the formalism in Ref.[19], we take the large size limit and expand ρ to linear order in B. As discussed there, the density matrix in real space basis can be decomposed into two parts, one of which is translationally invariant:

$$\rho_{r_1,r_2} = \bar{\rho}_{r_1,r_2} \exp(-i\vec{B} \cdot (\vec{r}_1 \times \vec{r}_2)/2), \tag{D.4}$$

where $\rho_{r1,r2}$ denotes the density matrix in position basis, and $\bar{\rho}$ is translation invariant. While the other part seems to be affected by the infinite range of $\mathbf{r}$, in our expression three ρ's appear together and the combination is short-ranged and can be expanded in B. It is thus straight forward to expand ρ explicitly and calculate.

In the following we apply the magnetic field in the z-direction and take ρ as a function of k_z, and $\vec{r}$ lies in the xy-plane. We take $\hbar = e = 1$. $\bar{\rho}$ has the following matrix elements up to first order in B:

$$\begin{aligned}
\langle\psi_{nk}|\bar{\rho}|\psi_{n'k'}\rangle &= \delta_{kk'}\left(\delta_{nn'} - \frac{1}{4}B\epsilon^{\gamma\delta}\mathcal{F}_{\gamma\delta,nn'}\right) \\
\langle\psi_{mk}|\bar{\rho}|\psi_{m'k'}\rangle &= \frac{1}{4}\delta_{kk'}B\epsilon^{\gamma\delta}\check{\mathcal{F}}_{\gamma\delta,mm'} \\
\langle\psi_{nk}|\bar{\rho}|\psi_{mk'}\rangle &= \delta_{kk'}\Big(\frac{i}{2}B\epsilon^{\gamma\delta}\frac{\langle\psi_{nk}|\{\partial_\gamma\rho_{0k},\partial_\delta H_k\}|\psi_{mk}\rangle}{E_{nk}-E_{mk}} \\
&\quad + \frac{\langle\psi_{nk}|H'_k|\psi_{mk}\rangle}{E_{nk}-E_{mk}}\Big);
\end{aligned} \tag{D.5}$$

note that the momentum here is two-dimensional and everything has implicit k_z, k_w dependence. n, n' are indices for occupied bands and m, m' are for empty bands. $\mathcal{F}$ is the nonabelian Berry curvature of the occupied bands,

$$\mathcal{F}_{\mu\nu} = \partial_\mu\mathcal{A}_\nu - \partial_\nu\mathcal{A}_\mu - i[\mathcal{A}_\mu,\mathcal{A}_\nu]; \tag{D.6}$$

similarly, $\check{\mathcal{F}}$ is the nonabelian field strength for the Berry's phase gauge field defined from the unoccupied bands:

$$\begin{aligned}
\check{\mathcal{A}}_{\mu,mm'} &= -i\langle u_{mk}|\frac{\partial}{\partial k^\mu}|u_{m'k}\rangle \\
\check{\mathcal{F}}_{\mu\nu} &= \partial_\mu\check{\mathcal{A}}_\nu - \partial_\nu\check{\mathcal{A}}_\mu - i[\check{\mathcal{A}}_\mu,\check{\mathcal{A}}_\nu].
\end{aligned} \tag{D.7}$$

In the following computation one would find these expressions useful:

$$\begin{aligned}
\mathcal{F}_{\mu\nu,nn'} &= -i\sum_m\langle\psi_{nk}|\partial_\mu|\psi_{mk}\rangle\langle\psi_{mk}|\partial_\nu|\psi_{n'k}\rangle \\
&\quad -(\mu\leftrightarrow\nu); \\
\check{\mathcal{F}}_{\mu\nu,mm'} &= -i\sum_n\langle\psi_{mk}|\partial_\mu|\psi_{nk}\rangle\langle\psi_{nk}|\partial_\nu|\psi_{m'k}\rangle \\
&\quad -(\mu\leftrightarrow\nu); \\
\epsilon^{\mu\nu\lambda\omega}\mathrm{Tr}(\mathcal{F}_{\mu\nu}\mathcal{F}_{\lambda\omega}) &= \epsilon^{\mu\nu\lambda\omega}\mathrm{Tr}(\check{\mathcal{F}}_{\omega\mu}\check{\mathcal{F}}_{\nu\lambda}).
\end{aligned} \tag{D.8}$$

Note that in the expression for the Berry's curvature $\mathcal{F}$, we use the whole Bloch wave function $|\psi\rangle$ instead of the periodic part $|u\rangle$ but here it makes no difference.

Now we start from Eq. D.1. Write explicitly in position basis, we have

$$\begin{aligned}\mathrm{Tr}\Big((\partial_\alpha\rho)\quad\rho\quad(\partial_\beta\rho)\Big) &= \int \mathrm{d}r_1\mathrm{d}r_2\mathrm{d}r_3(\partial_\alpha\bar{\rho}_{12})\bar{\rho}_{23}(\bar{\partial}_\beta\bar{\rho}_{31}) \\ &\quad \exp\left(-\frac{i}{2}B\epsilon^{\gamma\delta}(r_2-r_1)_\gamma(r_3-r_1)_\delta\right) \\ &= L_xL_y\int\frac{\mathrm{d}^2k'}{(2\pi)^2}\Big(\mathrm{Tr}\left((\partial_\alpha\bar{\rho})\bar{\rho}(\partial_\beta\bar{\rho})\right)\Big) \\ &+ \frac{i}{2}B\epsilon^{\gamma\delta}\mathrm{Tr}\left((\partial_\alpha\partial_\gamma\rho_0)\rho_0(\partial_\delta\partial_\beta\rho_0)\right)\Big) + \mathcal{O}(B^2),\end{aligned} \tag{D.9}$$

where in the second equality we taylor-expand in B, keep up to first order and go back to momentum space. We have also taken the infinite-size limit and make the sum of discrete momenta an integral. The trace on the right hand side traces over only the band indices.

The remaining task would be to plug in $\bar{\rho}$ and calculate explicitly to first order in B. One thing to notice is that when taking derivatives of $\bar{\rho}$, it acts not only on the matrix element but also on the basis. It is also useful to note that $\partial_u\rho_0$ only has non-vanishing matrix elements between the original occupied and empty states.

As we can see from Eq. D.5, the inter-gap and intra-gap matrix element of $\bar{\rho}$ look pretty different. Let us denote the former as ρ'. ρ' contributes only through the first term in the right hand side of Eq. D.9; since ρ' is already first order in B the remaining $\bar{\rho}$ can be replaced by ρ_0. Let $\rho' = A + A^\dagger$ with $A = (1-\rho_0)\rho'\rho_0$ (that is, A is the matrix element connecting occupied bands to empty bands and vice versa for $A^\dagger$), after explicit calculation, similar to Eq. D.3, we have

$$\begin{aligned}&\epsilon^{\alpha\beta}\left(\mathrm{Tr}(\partial_\alpha\rho'\rho_0\partial_\beta\rho_0) + \mathrm{Tr}(\partial_\alpha\rho_0\rho'\partial_\beta\rho_0) + \mathrm{Tr}(\partial_\alpha\rho_0\rho_0\partial_\beta\rho')\right) \\ =\ & -\partial_\alpha\left(\langle n|\partial_\beta|m\rangle A_{mn} - c.c.\right) \\ =\ & \partial_\alpha\mathrm{Tr}\left(\partial_\beta\rho_0(1-\rho_0)\rho'\rho_0 + h.c.\right);\end{aligned} \tag{D.10}$$

$|n\rangle$ is the short hand notation of $|\psi_{nk}\rangle$ and repeated indices are summed over.

Now that the inter-gap matrix elements are dealt with, the remaining part of the first term can also be expanded and calculated:

$$\epsilon^{\alpha\beta}\mathrm{Tr}(\partial_\alpha\bar{\rho}\bar{\rho}\partial_\beta\bar{\rho})|_{\text{remaining}} = \epsilon^{\alpha\beta}\Big(\frac{i}{2}\mathrm{Tr}(\mathcal{F}_{\alpha\beta})$$

$$
\begin{aligned}
&- \frac{3i}{8}\epsilon^{\gamma\delta}\mathrm{Tr}\left(\mathcal{F}_{\alpha\beta}\mathcal{F}_{\gamma\delta} - \check{\mathcal{F}}_{\alpha\beta}\check{\mathcal{F}}_{\gamma\delta}\right) \\
&+ \mathcal{O}(B^2)\Big). \qquad \text{(D.11)}
\end{aligned}
$$

The first term on the right hand side is proportional to B^0 and is similar to the polarization in 1D.

The only remaining part is the second term in Eq. D.9. This part proves to be somewhat tricky to calculate as one has to manually group terms into expressions of $\mathcal{F}$ and $\check{\mathcal{F}}$. Nevertheless, it is otherwise straight forward and one gets

$$
\begin{aligned}
\epsilon^{\alpha\beta}\ \epsilon^{\gamma\delta}\ \mathrm{Tr}(\partial_\gamma\partial_\alpha\rho_0\rho_0\partial_\delta\partial_\beta\rho_0) &= \\
\mathrm{Tr}\left(\frac{3}{4}\mathcal{F}_{\alpha\beta}\mathcal{F}_{\gamma\delta} - \frac{1}{4}\check{\mathcal{F}}_{\alpha\beta}\check{\mathcal{F}}_{\gamma\delta} + \check{\mathcal{F}}_{\delta\alpha}\check{\mathcal{F}}_{\gamma\beta}\right). & \qquad \text{(D.12)}
\end{aligned}
$$

Combining Eq. D.10, Eq. D.11, and Eq. D.12, and with the help of Eq. D.8 we get

$$
\begin{aligned}
\phi_{\text{Berry}} &= \int_S \mathrm{d}^2k \int_{BZ} \frac{\mathrm{d}^2k'}{(2\pi)^2} L_x L_y \epsilon^{\alpha\beta} \\
&\quad \Big[\epsilon^{\gamma\delta} B\mathrm{Tr}(-\frac{1}{4}\mathcal{F}_{\alpha\beta}\mathcal{F}_{\gamma\delta} + \frac{1}{2}\mathcal{F}_{\gamma\beta}\mathcal{F}_{\alpha\delta}) \\
&\quad -i\partial_\alpha \mathrm{Tr}(\partial_\beta\rho_{0k'}(1-\rho_{0k'})\bar{\rho}_{k'}\rho_{0k'} - h.c.)\Big]; \qquad \text{(D.13)}
\end{aligned}
$$

α, β span k_z, k_w and γ, δ span k_x, k_y. The integral of k' is performed on the 2D Brillouin zone in xy-plane. $\bar{\rho}_{k'} = \langle k'|\bar{\rho}|k'\rangle$ is the translationally invariant part of the density matrix at a given $(\vec{k}, k_w)$ and ρ_{0k} is the density matrix in zero field.

Notice that in Eq. D.13, the tensor structure in the first and the second term is different and we can rewrite the first term using the total-antisymmetric tensor in 4 dimensions:

$$
\begin{aligned}
\phi_{\text{Berry}} &= \phi_I + \phi_A \\
\phi_I &= \frac{-\Phi_B}{32\pi^2}\int_{S\times BZ} \mathrm{d}^4\mathbf{k}\epsilon^{abcd}\mathrm{Tr}(\mathcal{F}_{ab}\mathcal{F}_{cd}) & \text{(D.14)} \\
\phi_A &= \frac{-i\Phi_B}{4\pi^2}\int_{S\times BZ} \mathrm{d}^4\mathbf{k}\epsilon^{\alpha\beta}\partial_\alpha M_{\beta z} & \text{(D.15)} \\
M_{\alpha\beta} &= \mathrm{Tr}\left(\partial_\alpha\rho_{0k'}(1-\rho_{0k'})\frac{\partial\rho_{k'}}{\partial B^\beta}\rho_{0k'} - h.c.\right). & \text{(D.16)}
\end{aligned}
$$

We have explictly expanded the second term to first order in $\vec{B}$. a, b, c, d runs through all directions. Both integrals are total derivatives and we can integrate back to the boundary

which is the original 3D Brillouin zone:

$$\phi_I = \frac{-\Phi_B}{8\pi^2}\int \mathrm{d}^3k\epsilon^{abc}\mathrm{Tr}(\mathcal{A}_a\partial_b\mathcal{A}_c - i\frac{2}{3}\mathcal{A}_a\mathcal{A}_b\mathcal{A}_c) \tag{D.17}$$

$$\phi_A = \frac{-i\Phi_B}{4\pi^2}\int \mathrm{d}^3k M_{zz}. \tag{D.18}$$

ϕ_I is isotropic, i.e., independent of the direction of the applied magnetic field. ϕ_A, on the other hand, is anisotropic in the sense that if we do the same calculation for the magnetic field in x or y direction, the result in general would be different. Now we consider the gradual gauge transform in the i-direction and the magnetic field in the j-direction, the same calculation still goes through, provided that we take α, β in the i-direction and the extra direction, and γ, δ in the directions prependicular to the magnetic field. We get

$$\begin{aligned}\phi_{I,ij} &= \phi_I\delta_{ij};\\ \phi_{A,ij} &= \frac{-i\Phi_B}{4\pi^2}\int \mathrm{d}^3k M_{ij}.\end{aligned} \tag{D.19}$$

In terms of the effective theory, this means that the effective Lagrangian not only contains $\vec{E}\cdot\vec{B}$, in general we have $\sum_{ij}\alpha_{ij}E_iB_j$, where

$$\alpha_{ij} = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\left(\epsilon^{abc}\frac{-1}{2}\mathrm{Tr}(\mathcal{A}_a\partial_b\mathcal{A}_c - i\frac{2}{3}\mathcal{A}_a\mathcal{A}_b\mathcal{A}_c)\delta_{ij} + M_{ij}\right). \tag{D.20}$$

By calculating the Berry's phase of these processes, not only do we get the coefficient of the topological term but we also get a part which is a physical response which agrees with Ref. [19, 39]. In general $\sum_i M_{ii}$ also contributes to θ. If TR symmetry is present then $M_{ij} = 0$ and we see that the vacuum angle is shifted by π in the presence of the strong topological insulator.

Comparing to the derivation we have in Ch. 5, interestingly, the part that depends on energetics are separated out clearly. On the other hand, the remaining part is not obviously topologically invariant until explicitly summed over. As we have discussed in Ch. 6, the separation of the terms is more physical using the Green's functions.

Appendix E

Magneto-Electric Effect at Finite Momentum

In Ch, 6 we have argued heuristically that the trace of the ME tensor comes entirely from the surface, and therefore does not contribute at finite momentum. The locally measurable ME tensor is therefore traceless in the $q \to 0$ limit. We can directly calculate the ME tensor at finite q: Fourier transforming and expanding the hopping Hamitonian up to second order of A^μ, we have

$$\Delta H = \sum_{k,q} c^\dagger_{k+q/2} \partial_u H(k) c_{k-q/2} A^\mu(-q) + \frac{1}{2} \sum_{k,q,q'} c^\dagger_{k+(q+q')/2} \partial_u \partial_\nu H(k) c_{k-(q+q')/2} A^\mu(-q) A^\nu(-q'); \tag{E.1}$$

$H_k \equiv \sum_{d_i} t_{d_i} \exp(ikd_i)$ is a matrix. Integrating out the electrons, the effective action at quadratic order of A_μ reads

$$S_{\text{eff}} = \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{i}{2} A^\mu(q) A^\nu(-q) \mathrm{Tr}\Big(\partial_\mu \partial_\nu g^{-1}(k) g(k) + \partial_\mu g^{-1}(k) g(k + \frac{q}{2}) \partial_\nu g^{-1}(k) g(k - \frac{q}{2}) \Big); \tag{E.2}$$

similarly, the trace includes the integral of energy and momentum divided by 2π. The first term in the trace is from the second term in Eq. (E.1), usually called the paramagnetic current, and does not have q dependence. To compare with Eq. (6.2), we Taylor-expand the second term to second order in q to get the behavior in the $q \to 0$ limit: (From here on,

we drop the dependence on k to avoid cluttering.)

$$\begin{aligned} S_{\text{eff}} \sim & \int \frac{\mathrm{d}^4 q}{(2\pi)^4} - \frac{i}{8} q^\lambda q^\sigma A^\mu(q) A^\nu(-q) \\ & \mathrm{Tr}\Big(\partial_\mu g^{-1} \partial_\lambda g \partial_\nu g^{-1} \partial_\sigma g - \frac{1}{2} \partial_\mu g^{-1} \partial_\lambda \partial_\sigma g \partial_\nu g^{-1} g - \frac{1}{2} \partial_\mu g^{-1} g \partial_\nu g^{-1} \partial_\lambda \partial_\sigma g \Big) \\ & + \mathcal{O}(q^3); \end{aligned} \tag{E.3}$$

To further simplify the expression, let us now take the temporal gauge, $V = 0$. In the temporal gauge, we have to take either λ or σ to be in the time direction to have the expression contribute to the ME tensor. Since $\partial_i \partial_\omega g^{-1} = 0$, we can integrate-by-part the time derivative. using $\partial_\omega g = -g^2$, and rename the indices i, j, k, now running through only the spatial directions, we get

$$S_{ME} \sim \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{i}{2} \omega q^i A^j(q) A^k(-q) \mathrm{Tr}\Big(g \partial_j g^{-1} \partial_i g \partial_k g^{-1} g \Big). \tag{E.4}$$

Now we need to massage the expression a little bit. Let us use (ijk) as a short-hand notation of the expression $\mathrm{Tr}\Big(g \partial_i g^{-1} \partial_j g \partial_k g^{-1} g \Big)$. Integrating by parts[46], we have the following relation:

$$(ijk) + (jki) + (kij) = 0. \tag{E.5}$$

We therefore have

$$(jik) = \frac{1}{3}\big(2(jik) - (ikj) - (kji)\big). \tag{E.6}$$

In the trace in Eq. (E.4), only the part symmetric under the exchange of the index j and k would contribute, as we can change variables from q to $-q$, effectively exchanging $A^j(q)$ and $A^k(-q)$. Therefore, in the expression above, we can exchange j and k freely. We therefore have

$$\begin{aligned} S_{ME} \sim & \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{i}{6} \omega q^i A^j(q) A^k(-q) \big((jik) + (kij) - (ijk) - (kji) \big) \\ = & \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{i}{6} \omega q^i A^j(q) A^k(-q) \epsilon_{ij\ell} \epsilon_{ab\ell} \big((kab) + (bak) \big). \\ = & \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{i}{6} B^\ell(q) E^k(-q) \epsilon_{ab\ell} \big((kab) + (bak) \big) \\ \equiv & -\int \frac{\mathrm{d}^4 q}{(2\pi)^4} B^\ell(q) E^k(-q) \alpha_{k\ell}(q \to 0). \end{aligned} \tag{E.7}$$

$\alpha_{k\ell}(q \to 0) = -\frac{i}{6}\epsilon_{ab\ell}\big((kab) + (bak)\big)$ is traceless, as the two terms cancel each other with antisymmetrization.

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