Quantum field theoretic descriptions of topological phases in two and three dimensions

by

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A dissertation submitted in partial satisfaction of the requirements for the degree of Doctor of Philosophy in Physics in the Graduate Division of the University of California, Berkeley

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Abstract

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Topological phases of matter are purely quantum mechanical and have no classical analogue. Most phases in nature can be classified and studied classically through the concept of symmetry breaking and its theoretical description, Landau-Ginzburg field theory. In contrast to the general wisdom of Landau-Ginzburg field theory, the topological phases share the same symmetry as a trivial insulator and still are different phases. Having gapped spectrum in bulk, they support a metallic edge excitation robust against symmetry-respecting perturbation or an emergent fractional excitation in bulk. Following after fractional quantum Hall fluids, many topologically orderd phases, such as spin liquids and topological insulators, have been found and studied. Spin liquids are disordered phases of frustrated antiferromagnets and do not freeze and order even at the lowest temperature. They support an electrically neutral spin-$\frac{1}{2}$ excitation, which does not exist in a microscopic scale, with emergent dynamical gauge field in bulk and do not have an adiabatic path to a trivial paramagnet phase. The topological insulators are time-reversal symmetric band insulators which cannot evolve smoothly into a trivial insulator with the symmetry, and they have been intensely studied theoretically and experimentally for the last decade. Though the topological insulators are inherently non-interacting systems, they have exotic gapless edge and surface states which demonstrate many interesting quantum phenomena such as fractionalization, axionic electromagnetism, and half quantum Hall effect.

In this thesis, we study various quantum phenomena of the topological phases, mainly of the topological insulator and its close relatives in which the physics of spin liquids has been merged into. As they are intrinsically quantum many-body states, the quantum field theory is an invaluable tool to explore the venue of the phases and will be used thoroughly in this work.

First, we present a topological field theoretic description of the topological insulators and translational symmetric $\mathbb{Z}_2$ spin liquid. We demonstrate that abelian $BF$ theory is an effective field theory for the two and three dimensional topological insulators. We show that the phenomenologies of $BF$ theory are consistent with those of the topological insulators such as gapless edge and surface excitations and response functions to external gauge field. The same form of the $BF$ theory is also applicable to study the certain classes of $\mathbb{Z}_2$ spin liquids
with the gapless edge states. We closely examine the possible gapless edge theory of the BF theory and the translational symmetric spin liquids, and we show that the effective BF theories capture the bulk properties as well as the gapless edge spectrum of the spin liquid. Also we discuss the zero-temperature phase diagram of a thin film three dimensional topological insulators with two competing mass terms: time-reversal symmetric exciton condensation and time-reversal symmetry breaking Zeeman effect. There are two phases, quantum spin Hall phase and quantum anomalous Hall phase, and both phases support fractional excitations. We derive an effective topological field theory for the fractional excitations and examine the origin of the fractional excitations.

Next we consider the relatives of the topological insulators. First we discuss the proximate symmetry broken phases of topological Mott insulator, a U(1) spin liquid with fermionic spinons in the topological insulator state. The topologically non-trivial band structure of the spinon generates the axion term for the gauge field, and we show that the axion term changes the nature of the confined phase of the spin liquid. Contrast to the conventional confined phase which has only a bond order, the confined phase of the spin liquid is in general a coexisting phase of the two different orders: a current order and a bond order. We then consider another relative of the topological insulator: a bosonic symmetry protected topological phase in two dimensional space, with both PSU($N$) and time reversal symmetry. We develop an effective field theory for the phase, which is a SU($N$) principal chiral model with a $\Theta$-term, and reveal the physics of the topological phase in detail.

Finally we consider a topological semimetal, namely a Weyl semimetal. We first demonstrate that the Weyl semimetal can be realized in the magnetically doped topological band insulators. We explicitly derive the low energy theory of Weyl points from the general continuum Hamiltonian and tight-binding model of the topological insulators. Then we study superconducting instabilities of doped Weyl semimetals. We consider a minimal model for a Weyl semimetal and study the superconducting instabilities induced by a short-ranged attractive interaction. With the interaction, we find two competing states: a fully gapped finite-momentum pairing state and a nodal even-parity pairing state. We show that, in a mean field approximateion, the finite-momentum pairing state wins energetically against the usual even-parity paired state. We also show that exotic modes are localized at the full and half quantum vortices of the finite-momentum pairing state.
Dedicated to my father Youngsang Cho and my mother Sukyoung Kim,
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Chapter 1

Introduction

Most phases of matter in nature can be thoroughly studied and classified by Landau-Ginzburg theory. Landau-Ginzburg theory, based on symmetries, describes successfully the phases as well as transitions between them. However, new classes of the phases of strongly-interacting electrons, lying beyond the reach of Landau-Ginzburg theory, have been found following after the discovery of quantum Hall effects. The phases, named as ‘topological phases’ for fully gapped phases and ‘quantum phases’ for gapless phases\cite{1, 2}, include fractional quantum Hall effects, spin liquids, and topological insulators. Landau-Ginzburg theory, which distinguishes two different phases by their symmetries, is incapable of describing topological phases as two different topological phases may have the same symmetries. Due to the failure of Landau-Ginzburg approach, it is desirable to find other effective descriptions for those phases, and in particular a certain set of topological phases admits a (topological) field theoretic description. We can gain more intuition and knowledge about the phases by investigating the field theory.

In this introduction, we briefly review the physics of the primary examples of the topological phases and and their field theoretic descriptions.

1.1 Fractional quantum Hall effect

When electrons, confined to a two dimensional $xy$-plane, are exposed to magnetic field $B\hat{z}$ perpendicular to the plane, they experience Lorentz force $\propto \hat{z} \times \frac{d\vec{r}}{dt}$ and draw a simple circular orbit according to the classical Newtonian dynamics.

\begin{align}
\frac{m}{2} \frac{d^2 x}{dt^2} &= -\frac{eB}{c} \frac{dy}{dt}, \\
\frac{m}{2} \frac{d^2 y}{dt^2} &= \frac{eB}{c} \frac{dx}{dt}, \nonumber
\end{align}

\begin{equation}
z(t) = x(t) + iy(t) = C + \frac{iv_0 e^{i\omega_c t}}{w_c},
\end{equation}

\text{(1.1)}
Section 1.1. Fractional quantum Hall effect

such that $C$ and $v_0$ are the parameters determined by the initial condition, and $w_c = \frac{eB}{mc}$ is the cyclotron frequency. To obtain the quantum version of this cyclotron motion, we solve the Schrodinger equation by diagonalizing the Hamiltonian in the symmetric gauge $\vec{A} = B_2((-y, x, 0))$.

$$H = \left(-i\hbar \vec{\nabla} - \vec{A}\right)^2.$$ (1.2)

The set of the eigenstates of the Hamiltonian are called ‘Landau level’s labelled by the index $N \in \mathbb{Z}$, and they have a completely flat spectrum $E = \hbar w_c(N + \frac{1}{2})$, quantized in $\hbar w_c$. Note that there are two independent scales set by energy scale $\hbar w_c$ and length scale $l_B = \sqrt{\frac{\hbar c}{eB}}$ in the system.

Each Landau level contains $\frac{1}{2\pi l_B^2}$ single particle states per unit area, and the wavefunctions for the states can be obtained analytically. In particular the wavefunctions for the states in the lowest Landau level are,

$$\psi_m(z) = \frac{z^m \exp(-|z|^2/4l_B^2)}{\sqrt{2\pi l_B^2}} \prod_{i<j} (z_i - z_j) \exp\left(-\sum_i |z_i|^2/4l_B^2\right), \quad z = x + iy.$$ (1.3)

This many-body wavefunction is odd under the exchange of $z_i$ and $z_j$ as required by the fermionic statistics of electrons. Furthermore, the density of electrons $\propto |\Psi|^2$ is uniform in space and the wavefunction represents an incompressible state, $\kappa = -\frac{1}{V} \frac{\partial V}{\partial P} = 0$. Hence the quantum Hall effect is an electronic ‘fluid’ which does not freeze and crystalize at the lowest temperature.

Each filled Landau level contributes $\frac{\epsilon^2}{h}$ to the Hall conductance because each level contributes a single chiral mode at the boundary. Notice that as the energies of the levels are ‘quantized’, there will be an abrupt and ‘quantized’ change in the Hall conductance when the chemical potential crosses a Landau level. This phenomena is called integer quantum Hall effect as the Hall conductance is always an integral multiples of conductance quanta $\frac{e^2}{h}$.

For the given Hall response $\sigma_{xy} = \nu \frac{e^2}{h}$, we define $\nu$ as the filling of the Hall effect.

When the level is partially filled, one quickly notices that there is a huge degeneracy in the ground state. This degeneracy is removed when the interaction between electrons is included. The interaction removes the degeneracy in a very particular way [1,2], and it has been shown that only certain fractional fillings are allowed as stable incompressible quantum
Section 1.1. Fractional quantum Hall effect

Hall states.

\[ \sigma_{xy} = \frac{q e^2}{2p + 1 \hbar}, \quad p, q = 0, 1, 2, \cdots, \]  
(1.5)

Though different fillings have different physics, the most important and universal physics of those fractional quantum Hall effects can be understood by studying the \( \nu = \frac{1}{3} \) fractional quantum Hall state. So from here and below, we concentrate on the \( \nu = \frac{1}{3} \) fractional Hall state. This state is explained by the seminal work of Laughlin [3], and the wavefunction for \( \nu = \frac{1}{3} \) is,

\[ \Psi(z_1, z_2 \cdots z_n) \propto \prod_{i<j} (z_i - z_j)^3 \exp(- \sum_{i} |z_i|^2/4l_B^2). \]  
(1.6)

The Laughlin state features (1) a fractional excitation, defined as a ‘fraction’ of the underlying electron, of charge \( e/3 \) and statistical angle \( \theta = \pi/3 \) as can be seen from the plasma analogy of the wavefunction (1.6), (2) topological ground state degeneracy 3\( ^g \) on the manifold of genus \( g \), and (3) a single chiral mode living on the edge of the system. Notice that \( \Psi(z_1, z_2 \cdots z_n) \) in (1.6) cannot be written as a single Slater determinant, reflecting that the Laughlin state is a highly “entangled” state. Other fractionally filled Hall effects also demonstrate fractional excitations, topological degeneracy, and certain number of chiral (or achiral) edge modes.

Before proceeding to understand the physics of \( \nu = \frac{1}{3} \) state, we briefly pause and explain why fractional quantum Hall effects cannot be explained by a conventional Landau-Ginzburg theory. As the physics of integer quantum Hall effect and a fractional quantum Hall effect do not rely on the symmetry and both of the states can happen without any symmetry, Landau-Ginzburg theory dictates that two states belong to a single phase. On the other hand, two states definitely belong to the different phases; there is a fractional excitation (or topological degeneracy) in the fractional quantum Hall effect and is no such excitation (or degeneracy) in the integer quantum Hall effect. Thus the fractional quantum Hall effect is well beyond the reach of Landau-Ginzburg theory.

As Landau-Ginzburg theory fails to capture the physics of \( \nu = \frac{1}{3} \) state, we need to look for an effective description of the phase. Indeed there is a topological field theoretic description, known as U(1) Chern-Simons theory at level \( K \) [1, 2].

\[ L_{CS} = \frac{K}{4\pi} \epsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda - a_\mu j^\mu, \]  
(1.7)

with the compact U(1) gauge field \( a_\mu \sim a_\mu + 2\pi \) and the minimal coupling of the gauge field \( a_\mu \) to the source field \( j^\mu \) parametrizing the current of excitations in the fluid. There are several important features of the theory worth to comment.

First of all, the theory is a topological field theory. The action is invariant under the diffeomorphism or the coordinate transformation \( x_\mu \rightarrow x'_\mu \) and \( a_\mu \rightarrow \frac{\partial x'_\mu}{\partial x_\nu} a_\nu \). This implies that the phase described by the action is robust against any local perturbation (as the perturbation can be always scaled out) and also strongly independent of microscopic details. The action only cares the global geometry and topology where the phase is realized on. The way that the theory responds to this global information is to generate a topological
Section 1.1. Fractional quantum Hall effect

degeneracy \( K^g \), \( g \) is the genus of the system. We can exhibit the topological degeneracy by taking the mode expansion of the gauge fields on the torus \( T^2 = [0, L) \times [0, L) \). We choose a Coulomb gauge, where \( a_i, i = 1, 2 \) are physical and \( a_0 \) is a Lagrange multiplier, and consider no excitation inside the quantum Hall fluid \( j^\mu = 0 \). Expanding the Chern-Simons action, we reach to,

\[
L_{CS} = \frac{K}{4\pi} a_0 \varepsilon^{ij} \partial_i a_j + \frac{K}{4\pi} a_i \partial_0 a_j \varepsilon^{ij}.
\]  

(1.8)

By integrating out \( a_0 \), we obtain \( \varepsilon^{ij} \partial_i a_j = 0 \) and solve this equation by \( a_i = \frac{\alpha_i}{L} + \partial_i \phi \) with a spatially periodic scalar field \( \phi \) in the size of the tori \( L \) and spatially constant field \( \bar{a}_i \) (here \( \bar{a}_i \) is the “zero” mode of the gauge fluctuation). In terms of the new variables, we obtain the action on the torus.

\[
S_{CS} = \int d^2 x \int dt L_{CS} = \frac{K}{2\pi} \int dt \bar{a}_1 \partial_0 \bar{a}_2
\]  

(1.9)

The action implies a canonical commutation relation \([ \bar{a}_1, \bar{a}_2 ] = i \frac{2\pi}{K} \) and this generates an algebra for the two gauge invariant Wilson loop operators \( W_1 = \exp(i\bar{a}_1) \) and \( W_2 = \exp(i\bar{a}_2) \).

\[
W_1 W_2 = \exp(i \frac{2\pi}{K}) W_2 W_1
\]  

(1.10)

The minimum dimension of the representation of the above algebra is \( K \). Thus the action on the torus should involve at least \( K \) different quantum states, i.e., there are \( K \)-fold ground state degeneracy. By generalizing the above logic to the general manifold, one can show that each ‘handle’ generates \( K \)-fold ground state degeneracy and hence there will be \( K^g \)-fold ground state degeneracy on the manifold with the genus \( g \). Notice that two non-local operators \( (W_1, W_2) \) are involved to compute the topological degeneracy correctly. Any local perturbation that does not change the value of \( (W_1, W_2) \) would not change the degeneracy and this reveals a non-local feature of the topological phase.

Secondly we consider the excitation of the Chern-Simons action. By integrating out \( a_\mu \) in (1.7), we obtain an equation of motion.

\[
\frac{K}{2\pi} \varepsilon^{\mu\nu\lambda} \partial_\nu a_\lambda = j^\mu.
\]  

(1.11)

For a stationary single excitation \( j^0 = 1, j^i = 0 \), we see that the flux \( \frac{2\pi}{K} \) of \( a_\mu \) is bound to the excitation. Hence when a single excitation is rotated around the other excitation, the many-body wavefunction picks up the phase factor \( \exp \left( \frac{2\pi i}{K} \right) \), i.e., the excitation carries fractional statistics \( \theta = \frac{\pi}{K} \). To extract the electric charge of the excitation, we introduce non-dynamical external electromagnetic (or probe) gauge field \( A_\mu \) and coupled to the fields \( a_\mu \),

\[
L_{CS} = \frac{K}{4\pi} \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda - a_\mu j^\mu - \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu A_\lambda.
\]  

(1.12)

From the equation of motion (1.11), we see that \( j^\mu \) carries the electric charge \( \frac{1}{K} \). Given these information, we can easily guess that \( K = 3 \) should be the theory for the \( \nu = \frac{1}{3} \) fractional quantum Hall fluid.
Section 1.2. Topological band insulator

Thirdly we show that there is a chiral edge mode at the boundary of the phase. By considering a finite disk or a half infinite plane $M$ without excitation in the fluid, we have the Chern-Simons action in the Coulomb gauge $a_i = \partial_i \phi$ integrated up to the boundary $\partial M$.

$$S_{\partial M} = \int_M d^2 x dt L_{CS} = \int_{\partial M} dxdt \frac{K}{2\pi} \partial_x \phi(x,t) \partial_t \phi(x,t)$$  \hspace{1cm} (1.13)

This action has no Hamiltonian and it has a flat spectrum. This action simply implies that there is a canonical commutation relation $[\partial_x \phi(x',t), \phi(x,t)] = i \frac{2\pi}{K} \delta(x-x')$. In analogy with the Luttinger liquid theory, we can identify $\sim \frac{1}{2\pi} \partial_x \phi(x,t)$ as the excitation density $n(x,t)$. Physically the fluid will experience the potential well $\sim v n(x,t) n(x,t)$ at the boundary of the system and this translates into,

$$S_{\partial M} = \int_{\partial M} dxdt \frac{K}{2\pi} \left( \partial_x \phi(x,t) \partial_t \phi(x,t) - v(\partial_x \phi(x,t))^2 \right).$$  \hspace{1cm} (1.14)

The equation of motion for the $\phi$ field gives us $(\partial_t - v \partial_x) \phi = 0$ or $E = v k$ in the momentum space. Hence there is an excitation pole at $E = v k$ and the excitation propagates with the speed $v$. So there is a chiral edge mode with the fractional excitation $\sim \exp(i\phi)$ and the electron $\sim \exp(iK\phi)$.

Thus the simple U(1) Chern-Simons theory $^{[1.7]}$ at level $K$ faithfully captures the physics of fractional quantum Hall fluid at $\nu = \frac{1}{K}$. From the phenomenological approaches of fractional quantum Hall phases, e.g. composite fermion theory or parton theory, one can derive the Chern-Simons theory as the effective theory of the Hall effects and it explains why the Chern-Simons theory is so successful. We will show that another topological field theory is capable of describing topological insulators and some spin liquids in the chapter 4.

1.2 Topological band insulator

In the fractional quantum Hall states, the kinetic energy is quenched to zero due to the strong magnetic field and low temperature, and the interaction between electrons dominates the kinetic energy. Hence it is not so surprising, in some sense, to find an exotic topological phase in such a harsh situation (though it is still surprising of finding a fluid, not a solid). On the other hand in the most of common condensed matter systems, the opposite happens; the kinetic energy is dominant and the interaction is perturbative, and the physics is well described by the conventional band electron theory.

So one can ask if a topological phase can be realized in the absence of strong interaction or in the less harsh condition than the enviroment of the quantum Hall phases. Indeed, it has been shown that integer quantum Hall phase can arise in the honeycomb lattice without strong interaction and magnetic field $^{[4]}$, and later topological band insulator $^{[5-8]}$ is predicted and found in rather conventional materials with negligible interactions. They are topological phases in the sense that they do not have an obvious order parameter, which measures how much certain symmetry is broken, and exhibit gapless surface states, which
Section 1.2. Topological band insulator

are robust against symmetry-respecting perturbation. Instead of the order parameter, the wavefunctions carry a topological index which can be computed from the band structure of the phases. Notice that the topologically non-trivial insulator and trivial insulator are not so different in the bulk; both are simply gapped. The only difference between the topologically non-trivial and trivial phases manifests when we consider the boundary. The topological insulator, which is an abbreviation for the topologically non-trivial insulator, will support a gapless edge mode which cannot be gapped as far as the bulk remains gapped and certain symmetry is respected. This is different from a trivial electronic insulator; it can accidentally have a gapless dangling mode at the boundary, but the ‘gapless-ness’ of the mode is not robust in that it can be gapped if perturbation is included.

It is worth to comment that the topological band insulator in this section do not support fractionalization. So all the particle-like excitation in the low energy theory is an electron. This directly implies that the insulator will not have any topological degeneracy and always has a unique ground state. This does not mean that there is no interesting fractional excitation in the high energy spectrum; for example, the spin Hall effect can support a charge neutral spin carrying excitation $S_z = \pm \frac{1}{2}$ at the core of the magnetic vortex.

In this section, we will concentrate on those band insulators exhibiting topological phenomena and review the physics of the topological insulator. This section will introduce some terminologies and physics which are thoroughly used in chapter 3, chapter 5, and chapter 6 of this work.

1.2.1 From Haldane to Kane and Mele

Though the fractional quantum Hall effect requires a strong interaction, the integer quantum Hall effect can exist without interaction as it requires only the fully filled Landau levels. Then can we also remove the magnet field to have the integer quantum Hall phase? Haldane showed that it is possible. As the non-zero Hall effect requires the time-reversal symmetry broken, Haldane’s model [4] inevitably includes alternating magnetic fluxes, yet averaged to be zero. As the total flux is zero as well as interactions, one can ask where the topological nature of quantized Hall effect lives. In fact, the topological nature of the quantized Hall effect can be rephrased in terms of Berry connection and Berry flux over momentum space or the Brillouin zone (BZ), and the quantization comes from the quantized number of ‘magnetic monopole’, of the Berry connection, allowed in the BZ. So we can define a topological index, namely Thouless-Kohmoto-Nightingale-den Nijs (TKNN) integer or Chern number, for the topological phase.

The connection between the Chern number and the quantized Hall response manifests in the linear response theory of the band insulator. For the demonstration, we assume the lattice translational symmetry of the square lattice, $H(\vec{x} + \vec{R}) = H(\vec{x})$ for the lattice Hamiltonian $H(\vec{x})$ and any $\vec{R} = n\hat{x} + m\hat{y}$, $n, m \in \mathbb{Z}$, so that there is a well defined BZ = $(-\pi, \pi) \times (-\pi, \pi)$. We have chosen the square lattice for convenience but the discussion here is not dependent
on it. We can always find a Bloch wavefunction for the electron on such lattices.

\[ \psi_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r}), \]

with a periodic function \( u_{\vec{k}}(\vec{r} + \vec{R}) = u_{\vec{k}}(\vec{r}) \) under the lattice translation. By using the Bloch wavefunction as the basis, the Hall effect can be computed via a standard linear response theory at zero temperature and it can be shown that,

\[ \sigma_{xy} = \frac{ie^2}{2\pi\hbar} \int_{BZ} d^2k \left( \langle \partial_x u(k_x, k_y) | \partial_y u(k_x, k_y) \rangle - \langle \partial_y u(k_x, k_y) | \partial_x u(k_x, k_y) \rangle \right). \]

(1.16)

The quantity \( C = \frac{1}{2\pi} \int_{BZ} d^2k \left( \langle \partial_x u(k_x, k_y) | \partial_y u(k_x, k_y) \rangle - \langle \partial_y u(k_x, k_y) | \partial_x u(k_x, k_y) \rangle \right) \) has a name, Chern number, and is known to be quantized in mathematics. Also the Chern number \( C \) corresponds to the number of magnetic monopoles of the Berry connection \( \vec{A} = -i \langle u(k_x, k_y) | \partial u(k_x, k_y) \rangle \) in the band \( u(k_x, k_y) \) defined over the BZ. So each band carries a definite value of the Chern number or magnetic monopoles. This implies that as far as the bands are well separated in energy, the integer \( C \) cannot be changed because the monopole cannot vanish alone. The only way to change the number of the monopole (or the Chern number) contained by each band is to transfer monopoles from one band to another band, and it is necessary for the two bands to meet somewhere in the BZ to change their Chern numbers. Hence as far as the system remains gapped (or there is no band touching), the topological index can never be changed. Further investigation, relying on Laughlin’s argument, can show that this quantized Hall response is robust against interactions and disorders as far as the band gap is intact.

As a primary example of the topological phase based on the above theory, we discuss Haldane’s model. Haldane’s model consists of spinless electrons living on the honeycomb lattice at half filling, and no interaction between electrons.

\[ H = -t \sum_{<ij> \in N.N.} c_i^\dagger c_j + h.c. - t' \sum_{<ij> \in N.N.N.} (e^{i\phi_{i\rightarrow j}} c_i^\dagger c_j + h.c.) \]

(1.17)

The phase \( \phi_{i\rightarrow j} \) is \( \pm\phi \) such that \( \phi \in (0, 2\pi) \), depending on the link \( <ij> \). See the figure for the pattern Fig.1.1. The unit cell, containing two sublattices \( A \) and \( B \), for this model is generated by two unit vector \( \hat{a}_1 = (\frac{1}{2}, -\sqrt{3} \frac{1}{2}) \) and \( \hat{a}_2 = (\frac{1}{2}, \sqrt{3} \frac{1}{2}) \). The physics associated with the honeycomb lattice clearly manifests if we move to momentum space where the Hamiltonian is neatly written in terms of a two-component Dirac spinor (‘spinor’ here consists of ‘sublattice index’ \( A, B \) in the Honeycomb lattice).

\[ H(\vec{k}) = h_0(\vec{k})\sigma^0 + \sum_{a=1-3} h_a(\vec{k})\sigma^a \]

(1.18)
\[ h_0(\vec{k}) = 2t' \cos(\phi) \sum_{j=1,2} \cos(\vec{k} \cdot \hat{a}_j) \]

\[ h_1(\vec{k}) = t \sum_{j=1\ldots3} \cos(\vec{k} \cdot \hat{b}_j) \]

\[ h_2(\vec{k}) = t \sum_{j=1\ldots3} \sin(\vec{k} \cdot \hat{b}_j) \]

\[ h_3(\vec{k}) = 2t' \sin(\phi) \sum_{j=1\ldots2} \sin(\vec{k} \cdot \hat{a}_j) \] (1.19)

with \( \hat{b}_1 = (\frac{1}{2}, -\frac{1}{2\sqrt{3}}), \) \( \hat{b}_2 = (-\frac{1}{2}, -\frac{1}{2\sqrt{3}}), \) and \( \hat{b}_3 = (0, \frac{1}{3}) \). By defining a unit vector \( \hat{H} = (h_1, h_2, h_3)/\sqrt{\sum_a h_a^2} \), we can easily write down an expression for the Chern number of the Haldane model, given as the number of Skyrmions of \( \hat{H} \) over the BZ.

\[ C = \frac{1}{8\pi} \int d^2k \varepsilon^{ij} \dot{\hat{H}} \cdot \partial_i \hat{H} \times \partial_j \hat{H} \] (1.20)

It is not difficult to see that the Chern number \( C \) is \( \pm 1 \) as far as \( \phi \) is not 0 or \( \pi \), in which the system becomes time-reversal symmetric.

It is illuminating to consider the low-energy theory of Haldane’s model by expanding near the Dirac point \( K = (\frac{4\pi}{3}, 0) \) and \( K' = (-\frac{4\pi}{3}, 0) \) in BZ. Then we find a four-component massive Dirac theory.

\[ H = v\tau^3 \sigma \cdot \vec{k} + m\sigma^3, \] (1.21)

\( \tau^a \) is a Pauli matrix acting on the nodal index, \( \sigma^b \) is a Pauli matrix acting on the sublattice index, and \( m \sim t' \sin(\phi) \). Notice that \( m \) is a mass term (generating a band gap at the Dirac point) and is also time-reversal odd as \( T : \sigma^z \rightarrow -\sigma^z \) under time-reversal symmetry \( T = \tau^1 \sigma^3 K \) with the complex conjugation \( K \). For a massive two-component Dirac spinor \( H = v\sigma \cdot \vec{k} + m\sigma^z \), the Chern number is given as \( \frac{1}{2} \text{sgn}(m) \) [9]. For \( m \neq 0 \), we see that two Dirac points receive the band gap \( m \) with the equal sign and thus the total Chern number is \( \pm 1 \). This realizes the Hall phase with the quantized Hall response \( \pm \frac{e^2}{h} \). This implies that there is a chiral mode at the boundary.

\[ L = \psi^\dagger (i\partial_t - iv\partial_x) \psi \] (1.22)

The stability of the quantum Hall effect is guaranteed as there is no mass term for the chiral fermion \( \psi \). Equivalently there is no backscattering for the electrons simply because there is no counter propagating state.

The Dirac fermion theory \( H_{\text{kin}} = v\tau^3 \sigma \cdot \vec{k} \) admits only four different mass terms including quantum Hall mass \( \propto \sigma^z \). If we consider a spinful fermion on the honeycomb lattice and introduce a set of Pauli matrices \( S^\mu \) acting on the spin index, there are sixteen mass terms for the Dirac fermion \( H_{\text{kin}} = vS^0\tau^3 \sigma \cdot \vec{k} \). Among the sixteen masses, a particular mass
Figure 1.1: Haldane model. There are two sublattices \((A, B)\) in the honeycomb lattice. \(T_1\) and \(T_2\) represent unit translations \(\hat{a}_1\) and \(\hat{a}_2\) in the main text. The dashed line represents the second nearest neighbor hopping \(\propto t'\) in (1.17), and it represents \(t' \exp(i\phi)\) if an electron hops along the arrow and \(t' \exp(-i\phi)\) if an electron hops against the arrow.

Term \(\propto S^z \sigma^z\) is considered by Kane and Mele. The meaning of the mass ‘\(MS^z \sigma^z\)’ is clear; it generates band gap \(|M|\) with the opposite sign for the opposite spin states. Hence, for \(M > 0\), the spin-up fermion band carries the Chern number +1 and the spin-down fermion band carries the Chern number −1. This phase is named as “quantum spin Hall effect” due to the quantized spin-dependent Hall effect. Due to the Hall effect of the associated Chern number, there is a helical mode in which two gapless modes propagates to the opposite directions and each mode carries a definite \(S^z\)-quantum number.

\[
L = \psi^+_R(i\partial_t - iv\partial_x)\psi_R + \psi^+_L(i\partial_t + iv\partial_x)\psi_L, \quad S^z \psi = \pm \frac{1}{2} \psi, \quad (1.23)
\]

with + sign for \(\psi_R\), and − sign for \(\psi_L\) in the latter equation. Unlike the quantum Hall case (1.22), there is a natural mass term \(\sim \psi^+_R\psi_L + h.c.\) which can gap out the gapless
modes. So we ask when the helical mode is stable against the perturbation. Notice that the Hamiltonian has the $U(1) \times U(1)$ symmetry, one $U(1)$ is from the charge conservation and the other $U(1)$ is from $S^z$-conservation, and the mass term $\sim \psi_R^\dagger \psi_L + h.c.$ is not allowed if the symmetry is strictly required. Hence the spin Hall phase has a stable edge state as far as the $U(1) \times U(1)$ symmetry is respected. In other words, it is the symmetry that tunes the theory (1.23) critical and gapless.

Now we ask, by considering a multiple copies of the theory (1.23), how many different spin Hall phases are there.

$$L = \sum_{a=1}^{n} \psi_{a,R}^\dagger (i\partial_t - iv\partial_x)\psi_{a,R} + \psi_{a,L}^\dagger (i\partial_t + iv\partial_x)\psi_{a,L}. \quad (1.24)$$

All the right movers carry $S^z = \frac{1}{2}$ and all the left movers carry $S^z = -\frac{1}{2}$, and thus there cannot be a scattering between a right mover and a left mover. Thus any number of copies of the theory (1.23) is stable against any symmetry-respecting perturbation. Hence there are $\mathbb{Z}$ different spin Hall phases, and we say that there are $\mathbb{Z}$ classification for the $U(1) \times U(1)$ symmetry.

We can gain further knowledge about the phase by constructing a microscopic model for the phase [5]. By implementing a spin-dependent phase into Haldane model, one can easily realize such a model.

$$H = -t \sum_{<ij> \in N.N.} c_{i,\sigma}^\dagger c_{j,\sigma} + h.c. - t' \sum_{<ij> \in N.N.N.} (c_{i,\sigma}^\dagger [e^{iS^z\phi_{i\rightarrow j}}]^\sigma\tau c_{j,\tau} + h.c.) \quad (1.25)$$

The spin-dependent hopping term $\propto t'$ encodes a spin-dependent Lorentz force necessary for the spin Hall effect. The spin-dependent hopping term can be replaced with a more conventional spin-orbit coupling term.

$$H_{SOI} = -it' \sum_{<ij> \in N.N.N.} \nu_{ij} c_{i,\alpha}^\dagger [S^z]^\alpha\beta c_{j,\beta} + h.c., \quad (1.26)$$

with $\nu_{ij} = -\nu_{ji} = \pm 1$ depending on the link $<ij>$. This model realizes the spin Hall effect and has been studied by Kane and Mele [5].

However it is important to note that the term (1.26) is a part of the full spin-orbit coupling. In general the spin-orbit coupling will break the full rotational symmetry $SU(2)$ down to nothing and the realistic model would not have $S^z$-conservation. By remembering that all the important feature of the topological insulators is the existence of the gapless edge modes, one can ask if the edge modes can survive even without spin rotational symmetry by adding more spin-orbit coupling. In fact, it has been shown that the gapless edge modes survive even without the spin rotational symmetry as far as the time-reversal symmetry $\mathbb{Z}_2^T$ is respected [5, 10].

Fortunately the time-reversal symmetry is a common symmetry present in condensed matter systems, which is perhaps why the topological insulators are realized soon after the theoretical predictions, and this opens up a new class of the topological phases. In the following subsection we discuss the physics of the topological insulators protected by the time-reversal symmetry in details.
1.2.2 Time-reversal symmetric topological insulator

In this section we primarily discuss a topological non-trivial insulator with the time-reversal symmetry and we will call it as topological insulator for short in this subsection. We will review and remark important physics of the topological insulators \([5–7, 11–13]\) in two dimension and three dimension.

Two dimensional topological insulator

As explained in the previous subsection, there is a single non-trivial topological insulator in two dimension which supports an interesting gapless edge mode protected by the time-reversal symmetry. In fact, there are only two classes of time-reversal symmetric band insulators in two dimension; one is trivial and the other is non-trivial. So the classification for the time-reversal symmetric insulator in two dimension is \(\mathbb{Z}_2\). This is contrast to \(\mathbb{Z}\) classification for the spin Hall effect.

Below we consider the edge theory of two dimensional topological insulator and deduce the \(\mathbb{Z}_2\)-ness of the time-reversal symmetric insulator from the edge theory.

\[
L = \psi_R^\dagger (i\partial_t - iv\partial_x)\psi_R + \psi_L^\dagger (i\partial_t + iv\partial_x)\psi_L \tag{1.27}
\]

The only difference of the above equation from the spin Hall effect case (1.23) is that the fermions \((\psi_R, \psi_L)\) do not have a definite spin quantum number. Rather they transform non-trivially under the time-reversal symmetry \(T: \psi_R \rightarrow \psi_L\) and \(T: \psi_L \rightarrow -\psi_R\) so that \(T^2 = -1\) for the single particle states. Then one can show that the edge theory (1.27) can never be gapped without breaking \(\mathbb{Z}_2^T\) and the particle number conservation. On the other hand, we show the two copies of the topological insulator is trivial and prove that the classification is not \(Z\) but is \(\mathbb{Z}_2\) for general time-reversal symmetric insulators.

\[
L = \sum_{a=1,2} \left( \psi_{R,a}^\dagger (i\partial_t - iv\partial_x)\psi_{R,a} + \psi_{L,a}^\dagger (i\partial_t + iv\partial_x)\psi_{L,a} \right) \tag{1.28}
\]

with the time-reversal symmetry \(T: \psi_{R,a} \rightarrow \psi_{L,a}\) and \(T: \psi_{L,a} \rightarrow -\psi_{R,a}\). This theory can be gapped by the symmetry allowed term \(\sim \psi_{R,1}^\dagger \psi_{L,2} - \psi_{L,1}^\dagger \psi_{R,2} + h.c..\) In general if there are even number copies of the topological insulator, one can always find a symmetry-allowed mass term for the gapless modes. For the odd number copies of the topological insulators, all the modes can be gapped out except a single helical mode (1.27) so that any theory of the odd number of (1.27) belongs to the phase of the single copy theory (1.27). So there are only two phases for time-reversal symmetric band insulators in two dimension.

With the result above in hand, we can also claim a general stability of the edge theory via the fermion doubling theorem. The fermion doubling theorem dictates that any theory emergent from one dimensional lattice system with the time-reversal symmetry can never realize the theory (1.27) and it can have, at best, the double copied version (1.28) of the topological insulator. The edge theory of the topological insulator exists as the boundary
of the two dimensional theory and thus it can avoid the fermion doubling theorem. So whenever the topological insulator has a boundary with the vacuum and is coupled to any one dimensional mode or two dimensional trivial insulator, the helical edge theory will survive as far as the symmetry is respected.

We can define the topological index encoded in the wavefunction of the topological insulator. More precisely one can define a $\mathbb{Z}_2$ band index $D$ for the time-reversal symmetric band insulator [6, 14].

$$D = \frac{1}{2\pi} \left( \int_{\text{EBZ}} \kappa \cdot A(\kappa) - \int_{\text{EBZ}} d^2 F(\kappa) \right) \mod 2 \quad (1.29)$$

where $\vec{A}(\vec{k})$ and $F(\vec{k})$ are the Berry connection and curvature of the Bloch state $u(k_x, k_y)$, and ‘EBZ’ is the half of the BZ. Similar to the Chern number, the index cannot be changed as far as the band of the Bloch state $u(k_x, k_y)$ is well separated from the other bands. This implies that the topological nature of the insulator is robust as far as the insulator retains its band gap.

**Three dimensional topological insulator**

Surprisingly the index (1.29) in two dimension can be generalized to the $\mathbb{Z}_2$ index for three dimensional time-reversal symmetric insulators [6, 7] and implies that there is a single non-trivial topological insulator. This insulator supports a gapless surface mode living on the two dimensional boundary of the three dimensional insulator; there is a single two-component Dirac fermion on the surface.

$$H = \Psi^\dagger (i\vec{\partial} \cdot \vec{\sigma}) \Psi = \Psi^\dagger (i\partial_x \sigma^x + i\partial_y \sigma^y) \Psi \quad (1.30)$$

and $\vec{\sigma}$ are Pauli matrices acting on the spin index of the fermion. Then the time-reversal symmetry $T = i\sigma^y K$ can stabilize the Dirac fermion as the only mass term $\propto \sigma^z$ is not allowed by the time-reversal symmetry. As before one can deduce $\mathbb{Z}_2$-ness of the topological insulator from the Dirac theory (1.30) by considering the multiple copies of it.

The Dirac fermion theory (1.30) on the boundary of the bulk insulator can be gapped when the time-reversal symmetry is broken. Then the surface theory supports a half-quantum Hall effect due to the non-zero Chern number $C = \frac{1}{2} \text{sgn}(m)$ associated with the mass term $m\sigma^z$. Notice that the half Chern number is not allowed for the purely two dimensional lattice systems; this is another occasion where the boundary of the $D$-dimensional topological phase is different from pure $(D-1)$-dimensional theory.

The half quantum Hall effect on the boundary can be written in terms of the non-compact electromagnetic field $A_\mu$ over the boundary $\partial M$ [6, 13, 14].

$$L = \frac{1}{8\pi} \int_{\partial M} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda = \frac{1}{8\pi} \int_M \varepsilon^{\mu\nu\lambda\rho} \partial_\mu A_\nu \partial_\lambda A_\rho \quad (1.31)$$
The above Lagrangian $\propto \int_M \partial A \partial A$ has its name, axion term [15]. It has a long history in the particle physics and is considered to solve the $CP$-problem in a non-abelian gauge theory and associated oblique confinement [16]. The axion term is the origin of many anomalous physics of the three dimensional topological insulator which is part of this thesis. So here we do not get into the details of all the phenomenologies associated with the axion term (1.31) but we discuss only one anomaly physics in this introduction [17].

When the surface of the topological insulator is gapped by breaking the time-reversal symmetry only on surface, the topological insulator and a trivial insulator seem to belong to the same phase. However the bulk of the topological insulator still respects the time-reversal symmetry and the topological phase itself should be well defined even without the surface. Then one can ask if we can sharply distinguish, the topological insulator with the gapped surface state and a trivial insulator by looking at the bulk. Indeed one can make a distinction by looking at the statistics of the electrically neutral magnetic monopole in the bulk; the neutral monopole is bosonic in the trivial insulator and is fermionic in the topological insulator. This difference is traced back to the axion term (1.31). The axion term (1.31) dresses the $4\pi$-magnetic monopole with the polarization charge $e$ while keeping the statistics bosonic (See the chapter 6 and references therein for the detailed argument), and thus it needs to absorb an electron to become electrically neutral. Because the electron is fermionic and there is no additional statistical transmutation for the bound state of a unit charge and $4\pi$ magnetic monopole, the neutral magnetic monopole in the topological insulator should be fermionic. This effect is named as ‘statistical anomaly’ [17].

1.2.3 Intrinsic topological order vs. symmetry protected topological order

We have seen that the time-reversal symmetric topological insulator is not different from the trivial insulator if the time-reversal symmetry is removed. In fact it is the symmetry that tunes edge or surface theory critical. So if the symmetry is violated, the edge and bulk of the topological insulator can adiabatically evolve into a trivial atomic insulator. In other words, the topological distinction is a working definition if there is the symmetry. This is different from the fractional quantum Hall phase where we do not need a symmetry to make a distinction from a trivial atomic insulator. All the symmetry can be broken in the fractional quantum Hall phase and the phase is still different from a trivial insulator because of the fractional excitations and associated topological degeneracy.

We define an intrinsic topological phase [1, 2, 18], a gapped phase with an intrinsic topological order, as the phase which does not rely on a symmetry and cannot be smoothly evolved into a trivial insulator without a phase transition. It includes, for example, fractional quantum Hall phases and spin liquids. Those phases typically involve a fractional excitation and topological degeneracy on topologically non-trivial manifolds. The intricate physics of the phases are patterned into the quantum wavefunctions, and the wavefunction cannot be unwinded into that of the trivial insulator without passing through a phase transition,
marking a distinction of the topological phases from the trivial phase.

On the other hand, we define a symmetry protected topological phase \cite{18} as the gapped phase which is different from a trivial insulator only when certain symmetry is present in the system. Otherwise it is no longer different from a trivial insulator. It includes, for example, a spin Hall phase and time-reversal symmetric topological insulators. Those phases do not support any fractional excitation but a gapless edge and surface mode tuned to the criticality by the symmetry.

Both intrinsic topological phases and symmetry protected topological phases are topologically ordered in the sense that there is no obvious order parameter in the sense of Landau-Ginzburg theory.

1.2.4 Beyond topological band insulators

The topological insulator is just one symmetry protected topological phase, and there are many other different symmetry protected topological phases for the electrons and bosons. For example there are ten primary classes \cite{19,20}, classified by chiral symmetry, time-reversal symmetry, and particle-hole symmetry, of the electronic insulators and superconductors in $D$-dimensions. If the classification with certain symmetry is beyond 1, there is always at least one non-trivial topological phase respecting the symmetry. For example, for the three dimensional Hamiltonian with the particle-hole symmetry and time-reversal symmetry, there is $\mathbb{Z}_2$ classification and this means that there is a single non-trivial superconductor with fully gapped bulk spectrum. This superconductivity is usually called as the time-reversal symmetric topological superconductor or topological superconductor for short. This superconductor supports a gapless Majorana surface mode at its boundary,

$$L = \Psi^T (i \partial_x \sigma_x + i \partial_y \sigma_y) \Psi, \quad \Psi^* = \Psi.$$  \hfill (1.32)

As like the topological insulator, the surface state is protected by the time-reversal symmetry. There have been many studies on this exotic superconductor and they are not only the theoretical pursuit; it is expected to emerge as one of the most competing states in the doped topological insulator \cite{21}. There are a few superconducting materials with the strong spin-orbit coupling and they are suspected to be the topological superconductor.

Also the symmetry protected topological phase does not need to be fermionic, and there are non-trivial bosonic symmetry-protected topological phases \cite{18,22}. The non-trivial bosonic phase is also gapped in bulk and supports a gapless edge or surface mode. This phase is different from the usual Mott insulator and the superfluid phase of the bosons. We will construct one explicit example in the chapter \ref{ch:topological}

**topological semimetal**

So far we have concentrated on the gapped phases with exotic edge modes and tried to classify the gapped phases according to the topological nature of wavefunctions. We now
consider a stable ‘gapless’ phase which is protected by the topological nature and lattice symmetry [23]. To illustrate this, let us consider the following two-band model Hamiltonian.

\[ H = \sigma^x \sin(k_x) + \sigma^y \sin(k_y) + M \sigma^z (2 - \cos(k_x) - \cos(k_y)) + m \sigma^z (\cos(k_z) - \cos(Q)), \] (1.33)

with \( Q \neq 0 \) and \( m, M \neq 0 \), and \( \sigma^\mu \) is the Pauli matrix acting on the spin index of the underlying fermions. There are two nodes at \( \vec{k}_c = (0, 0, \pm Q) \) in the spectrum, and we expand the Hamiltonian to see the low-energy physics near a node \( (0, 0, Q) \).

\[ H \approx \sigma^x k_x + \sigma^y k_y + v_z \sigma^z \delta k_z, \quad \delta k_z = k_z - Q, v_z = -m \sin(Q) \] (1.34)

The theory is manifestly relativistic, and it is known as the Weyl fermion in the high energy physics context. The semimetal with the Weyl-like node is called ‘Weyl semimetal’. As the low-energy Hamiltonian (1.34) involves all of the three Pauli matrices, it is impossible to generate the gap. The only way to generate the mass gap is to introduce a perturbation connecting the node at \( (0, 0, Q) \) to the other node at \( (0, 0, -Q) \). If there is a lattice translational symmetry and \( Q \) is not commensurate, then such perturbation can not present and the node is guaranteed to be stable. The stability can be further illustrated if one notices that the Weyl node is a \( 2\pi \) monopole for the Berry connection centered at \( (0, 0, Q) \). As the monopole cannot disappear alone, the monopole or the node will survive as far as it does not encounter an anti-monopole [23]. Also the non-zero monopole of Berry connection means a non-zero Chern number in the system. This directly implies that the Weyl semimetal will carry a non-zero Hall effect [24] in the three dimensional bulk. On the other hand by diagonalizing the Hamiltonian (1.33) with the boundary, one can show that there is a flat band on the surface, again protected by the lattice translational symmetry.

The model Hamiltonian is explicitly breaking time-reversal symmetry and has a strong spin-orbit coupling. This clues us that the phase might show up in the other conventional systems with the strong spin-orbit coupling and the broken time-reversal symmetry. Indeed, it can show up in the iridates [24, 25], or topological insulator materials [26, 27] as illustrated in the chapter 8.

1.3 Spin liquid

In this section we turn our attention from electronic phases to the frustrated antiferromagnets, which has been one of the central subjects of condensed matter physics. In particular we concentrate on a fluid-like disordered phase, namely a spin liquid phase [28–30], of the interacting spins. The spin liquid phase supports a deconfined fractional excitation at its low energy spectrum as like fractional quantum Hall fluids. Contrast to the natural excitation in the spin system carrying spin-1, which corresponds to flipping a spin, the fractional excitation is a fraction of the underlying spin in that it carries spin-\( \frac{1}{2} \) and this excitation is named as spinon. The fractionalization does not come alone and it involves a dynamical gauge theory coupled to the spinon.
There are many interesting details in this subject but we will restrict ourselves to a few aspects of the phase, the gauge theory and its confined phase associated with the spin liquid, and the “projective symmetry group” analysis which are extensively used in chapter 4 and chapter 6 of this work.

1.3.1 Mean field theory for spin liquids

We review the mean field theory for spin liquids and will closely follow the reference [31, 32]. The Hamiltonian we concern about is the spin Hamiltonian,

\[ H = \sum_{<ij>} J_{ij} \hat{S}_i \cdot \hat{S}_j, \]  

where the fractional excitation is not seen apparently. We want to access a completely symmetric, or completely disordered, phase with the fractionalization if there is any of such phase from the spin Hamiltonian. To access such a phase, we introduce fermionic fields \( f_{i,\alpha} \) carrying a spin index and write the spin operator in terms of the fermionic field \( f_{i,\alpha} \).

\[ \hat{S}_j = \frac{1}{2} f_{j,\alpha}^\dagger \sigma^{\alpha\beta} f_{j,\beta}, \quad f_{j,\alpha}^\dagger f_{j,\alpha} = 1. \]  

(1.36)

We plug (1.36) into the parent Hamiltonian (1.35) and end up with the four fermion terms with the hard constraint \( f_{j,\alpha}^\dagger f_{j,\alpha} = 1 \) for the new variables \( f_\sigma \).

\[ H_{\text{exact}} = \sum_{ij} \left[ -\frac{J_{ij}}{2} f_{i,\sigma}^\dagger f_{j,\sigma} f_{j,\tau}^\dagger f_{i,\tau} + J_{ij} \left( \frac{n_i}{2} - \frac{n_i n_j}{4} \right) \right], \quad f_{j,\alpha}^\dagger f_{j,\alpha} = 1. \]  

(1.37)

We cannot solve this Hamiltonian exactly as we do not know how to diagonalize the Hamiltonian where four fields are interacting. So we make several approximations to make it tractable.

First of all, we soften the hard constraint \( f_{j,\alpha}^\dagger f_{j,\alpha} = 1 \) by introducing Lagrange multiplier \( a_0(i) \) and add a term \( \sum_j a_0(j)(f_{j,\sigma}^\dagger f_{j,\sigma} - 1) \) to the Hamiltonian (1.37). On integrating out \( a_0(j) \), we restore the constraint at every site.

Second, we introduce a pair of the Hubbard-Stratonovich fields to decouple the four fermion term in (1.37) into the quadratic mean-field Hamiltonian.

\[ \chi_{ij} = \chi_{ji}^\dagger = 2 \langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle, \quad \eta_{ij} = \eta_{ji} = -2 \langle f_{i,\alpha} f_{j,\beta} \varepsilon^{\alpha\beta} \rangle \]  

(1.38)

The mean-field parameters are chosen in a way that the spin rotational symmetry is not broken explicitly. If one looks for the state without the spin rotational symmetry, more mean field parameters should be considered. On plugging these mean-field parameters, we obtain the mean-field Hamiltonian for the exact Hamiltonian (1.37),

\[ H_{\text{MF}} = \sum_{ij} \frac{3 J_{ij}}{8} \left[ \chi_{ij} f_{i,\sigma}^\dagger f_{j,\sigma} + \eta_{ij} f_{i,\sigma} f_{j,\tau} \varepsilon^{\sigma\tau} + \text{h.c.} - |\chi_{ij}|^2 - |\eta_{ij}|^2 \right] + \sum_j a_0(j)(f_{j,\sigma}^\dagger f_{j,\sigma} - 1). \]  

(1.39)
which is exactly solvable. By diagonalizing the Hamiltonian (1.39), one obtains set of bands parameterized by \((\chi_{ij}, \eta_{ij})\) and a wavefunction \(|\Psi_{MF}(\chi_{ij}, \eta_{ij})\rangle\) by filling the bands up to the zero energy. Then one can ask how good the mean field wave function \(|\Psi_{MF}(\chi_{ij}, \eta_{ij})\rangle\) is. This is obtained by projecting \(|\Psi_{MF}(\chi_{ij}, \eta_{ij})\rangle\) to the state of one fermion per site and measure the energy with respect to the parent Hamiltonian \(H_{exact}(1.37)\) or equivalently to the spin Hamiltonian (1.35).

\[
E_{MF} = \langle \Psi_{MF}(\chi_{ij}, \eta_{ij}) | P H_{exact} P | \Psi_{MF}(\chi_{ij}, \eta_{ij}) \rangle,
\]

where \(P\) is the projection operator to make \(f_{j,\alpha}^\dagger f_{j,\alpha} = 1\) strictly satisfied. If \(E_{MF}\) is better than energy of any other known spin states and valence bond solid phases, then indeed the spin liquid state, the exotic state with a fractional excitation, can be potentially the ground state of the spin Hamiltonian (1.35)!

The last step is to check the stability of the mean-field state which involves the gauge theory.

Before discussing the stability, we pause and consider the gauge redundancy of the naive mean-field description (1.39), and then we are naturally led to the projective symmetry group analysis which effectively encodes the (lattice) symmetries into the spin liquid.

### Gauge redundancy

Where does the gauge theory kick in to the theory? this is traced back to the change of variables (1.36) we have made for the spin operator. Notice that the spin operator and the constraint in (1.36) are invariant under the local gauge transformation \(G : f_j \rightarrow \exp(i\phi_j) f_j\) for the fermion operators [31, 32].

Under the \(U(1)\) gauge transformation, the mean field Hamiltonian with \(\eta = 0\) is invariant because \(G : \chi_{ij} \rightarrow \exp(i(\phi_i - \phi_j)) \chi_{ij}\). Thus if \(\eta = 0\), we can introduce a \(U(1)\) gauge field \(a_{ij}\), minimally coupled to the fermions, living on the link \((i,j)\) such that \(\chi_{ij} = e^{ia_{ij}}|\chi_{ij}|\), and the gauge transformation acts as the usual lattice version of the electromagnetism \(G : a_{ij} \rightarrow a_{ij} + \phi_i - \phi_j\). Then \(a_{ij}\) is non-dynamical at this stage. However it becomes a dynamical field in the low-energy theory as it acquires dynamics upon integrating out the high-energy fermions in the renormalization sense. Thus the low energy theory will be described by the usual electromagnetism.

\[
L = \frac{1}{2\pi g} (\varepsilon^{\mu\nu\lambda} \partial_\nu a_\lambda)^2 \propto \vec{E}^2 - \vec{B}^2
\]

The spin liquid with the \(U(1)\) gauge redundancy is called \(U(1)\) spin liquid. For the \(U(1)\) spin liquid, it is often important to remember that the gauge field \(a_{ij}\) is compact \(a_{ij} \sim a_{ij} + 2\pi\) as it has started from the lattice gauge theory and the compactness allows a monopole excitation in the spin liquid, which is crucial for the fate of the gauge theory as we will review soon.

If \(\eta_{ij}\) is non-zero, then the mean-field Hamiltonian explicitly breaks the \(U(1)\) gauge rotation. However there is a residual \(\mathbb{Z}_2\) gauge degree of freedom such that for \(G : f_i \rightarrow s_i f_i, s_i = \pm 1\) and \(G : (\chi_{ij}, \eta_{ij}) \rightarrow (s_i \chi_{ij} s_j, s_i \eta_{ij} s_j)\). As like the \(U(1)\) case, \(\mathbb{Z}_2\) gauge field will be dynamical in the low-energy. Also the spin liquid with the \(\mathbb{Z}_2\) gauge redundancy is called \(\mathbb{Z}_2\) spin liquid.
We have discussed only U(1) and \( \mathbb{Z}_2 \) spin liquids but the U(1) gauge redundancy can be extended to SU(2) gauge symmetry, by mixing U(1) gauge symmetry with the \( \mathbb{Z}_2 \) particle-hole symmetry, for the fermionic spinon. Also we could have started with the bosonic field \( z_{i,\sigma} \), instead of the fermionic variable \( f_{j,\sigma} \), for the spin operator.

\[
\hat{S}_j = \frac{1}{2} z^\dagger_{j,\alpha} \hat{\sigma}^{\alpha\beta} z_{j,\beta}, \quad z^\dagger_{j,\alpha} z_{j,\alpha} = 1
\]  

(1.42)

For the bosonic spin liquids, the possible gauge groups are U(1) and \( \mathbb{Z}_2 \).

**Projective symmetry group**

We now discuss complication induced [31, 32] by the gauge redundancy of the mean field description. The mean field Hamiltonian (1.39) and the mean field state \( |\Psi_{MF}(\chi_{ij}, \eta_{ij})\rangle \) might look different from another mean field Hamiltonian and state \( |\Psi_{MF}(\tilde{\chi}_{ij}, \tilde{\eta}_{ij})\rangle \). However, they might turn out to be the same state by a proper gauge transformation.

Thus to avoid this complication, it is desirable to fix the gauge and classify the mean field Hamiltonian in a gauge invariant way. The systematic method to accomplish this is called projective symmetry group, and we require the mean field Hamiltonian (1.39) invariant under the symmetry operation followed by the gauge rotation. In particular this projective symmetry group analysis allows us to encode the symmetries to the spin liquid state as we look for a completely symmetric spin liquid. For example, we consider a translational symmetric \( \mathbb{Z}_2 \) spin liquid where the translational symmetry in 2D is generated by two unit lattice translation operators \( T_x \) and \( T_y \). \( T_x \) and \( T_y \) satisfy an algebraic relation.

\[
T_x T_y = T_y T_x
\]  

(1.43)

This implies that the translational symmetric mean field Hamiltonian (1.39) should satisfy the following,

\[
G_x T_x G_y T_y = \pm G_y T_y G_x T_x,
\]  

(1.44)

where \( \pm 1 \) on the right hand side comes from the \( \mathbb{Z}_2 \) gauge degrees of freedom for the spin liquid. Thus by requiring the translational symmetry, we obtain two different \( \mathbb{Z}_2 \) spin liquid phases, one for \( +1 \) sign, and the other for \( -1 \) sign. By requiring all the possible symmetries and considering all the possible algebraic relations between the symmetry operations, we can classify how many symmetric spin liquid phases can be there. For example, there are at most 196 different fermionic \( \mathbb{Z}_2 \) spin liquid states [31] on the square lattice with the full lattice symmetry if we consider only the ‘matter field’ \( f_{i,\sigma} \).

As a concrete practice for the projective symmetry group analysis, we will show that there are only two possible different \( \mathbb{Z}_2 \) vison states in Kagome lattice (vison is a vortex excitation in a \( \mathbb{Z}_2 \) spin liquid).
Example: only two different vison states in Kagome lattice

Visons are the magnetic excitation in the $\mathbb{Z}_2$ gauge theory. The vison lives in the dual lattice of the original lattice and is minimally coupled to the dual $\mathbb{Z}_2$ gauge theory. The vison can be represented as the Ising degree $\tau(x, y) = \pm 1$ of freedom at the dual site $(x, y)$. Here we particularly consider the $\mathbb{Z}_2$ spin liquid on the Kagome lattice. Powerful numerical methods, namely density matrix renormalization group method [33, 34], have found a $\mathbb{Z}_2$ spin liquid state recently, and it has been shown that an interesting valence bond solid phase is sitting right next to the spin liquid. By noticing that the natural way to access the valence bond solid phase from the spin liquid is to condense the vison in the spin liquid (see the chapter 1.3.2 for the detailed reasoning for this statement), we ask how many different vison states are available in a $\mathbb{Z}_2$ spin liquid on Kagome lattice. We will show that there are only two different possible states for the Ising vison fields by performing the projective symmetry group analysis.

As the vison would not carry the spin quantum number, it is enough for the vison to consider only the lattice symmetries of Kagome lattice, generated by $\{T_1, T_2, \sigma, R\}$. The dual lattice has three sublattices $\{A, B, C\}$, and we parametrized the site $(x, y)$ as $x(1, 0) + y(-\frac{1}{2}, \frac{\sqrt{3}}{2})$ in Cartesian coordinate. See the figure 1.2 for the symmetry operations and the dual lattice. First we identify how they act on the dual lattice.

$$
T_1 : (x, y) \rightarrow (x + 1, y) \\
T_2 : (x, y) \rightarrow (x, y + 1) \\
\sigma : (x, y)_A \rightarrow (y, x)_A \\
(x, y)_B \rightarrow (y, x)_C \\
(x, y)_C \rightarrow (y, x)_B \\
R : (x, y)_A \rightarrow (x - y, x)_A \\
(x, y)_B \rightarrow (x - y, x)_C \\
(x, y)_C \rightarrow (x - y - 1, x)_B
$$

There are eight different algebraic relations for the symmetry operations $\{T_1, T_2, \sigma, R\}$.

$$
T_1 T_2 (T_1)^{-1} (T_2)^{-1} = 1 \\
T_1 \sigma (T_2)^{-1} \sigma^{-1} = 1 \\
T_2 \sigma (T_1)^{-1} \sigma^{-1} = 1 \\
\sigma^2 = 1 \\
R \sigma R \sigma = 1 \\
T_1 R T_2 (R)^{-1} = 1 \\
T_2 R (T_2)^{-1} (T_1)^{-1} (R)^{-1} = 1 \\
R^6 = 1
$$
As there are eight different algebraic equations and we are considering $\mathbb{Z}_2$ gauge theory, naively one might expect that there are $2^8 = 256$ different possible projective symmetry groups. The symmetry relation (1.46) generates the following algebraic equations for the
gauge transformations.

\[ G_1 T_1 G_2 T_2 (G_1 T_1)^{-1} (G_2 T_2)^{-1} = s_1, \]
\[ G_1 T_1 G_\sigma \sigma (G_2 T_2)^{-1} G_\sigma \sigma^{-1} = s_2, \]
\[ G_2 T_2 G_\sigma \sigma (G_1 T_1)^{-1} G_\sigma \sigma^{-1} = s_3, \]
\[ G_\sigma \sigma G_\sigma \sigma = s_4, \]
\[ G_R G_\sigma \sigma G_R R\sigma = s_5, \]
\[ G_1 T_1 G_R G_2 T_2 (G_R R)^{-1} = s_6, \]
\[ G_2 T_2 G_R G_2 T_2 (G_R R)^{-1} (G_1 T_1)^{-1} (G_R R)^{-1} = s_7. \]
\[ (G_R R)^6 = s_8, \quad (1.47) \]

with \( s_i = \pm 1, i = 1, 2, \ldots, 8 \). We look for a set of gauge transformations \{\( G_1, G_2, G_\sigma, G_R \)\}, as the function of the space coordinate \((x, y; p)\) with the sublattice index \( p = A, B, C \), satisfying \((1.47)\). To solve the equations, we notice that \( X^{-1} G_S(x, y) X = G_S(X(x, y)) \) where \( X \) and \( S \) are the symmetry operations. For example, let us solve the first equation of \((1.47)\). We first choose \( G_1 = 1 \) as a gauge choice. Then we have,

\[ T_1 G_2 (x, y) T_2 (T_1)^{-1} (T_2)^{-1} (G_2 (x, y))^{-1} = s_1 \rightarrow T_1 G_2 (x, y) (T_1)^{-1} G_2 (x, y) = s_1, \quad (1.48) \]

where we used the facts \( T_1 T_2 (T_1)^{-1} (T_2)^{-1} = 1 \) and \( G^{-1} = G \) in the Ising \( \mathbb{Z}_2 \) gauge theory. Now the equation reads \( G_2 (x-1, y) G_2 (x, y) = s_1 \rightarrow G_2 (x, y) = (s_1)^x \) up to the gauge choice. Similarly we can solve the eight equations and we present the solution of the equations \((1.47)\).

\[ G_1 (x, y) = 1, \]
\[ G_2 (x, y) = (s_1)^x, \]
\[ G_\sigma (x, y) = (s_1)^{xy+x+y}, \]
\[ G_R (x, y) = (s_1)^{x+y+xy+(x(x+1)+y(y+1))/2}(s_5)^{x+y}, \quad (1.49) \]

and \( s_1 = s_2 = s_3, s_4 = 1, s_5 = s_6, \) and \( s_8 = 1 \) to be consistent with the ising \( \mathbb{Z}_2 \) gauge theory. It looks like that there are four different vison states from \((s_1 = \pm 1, s_5 = \pm 1)\), but \( s_1 \) should be \(-1\) to capture the Berry phase of the vison when it encircles one direct lattice site (this is because of the mutually semionic statistics of the spinon and the vison in the \( \mathbb{Z}_2 \) spin liquid). Hence the only independent sign is \( s_5 = \pm 1 \) and hence there are only two different possible projective symmetry groups for the vison on the Kagome lattice, which is rather surprising if we compare it to the case of the 196 different \( \mathbb{Z}_2 \) spin liquid states on the square lattice.

1.3.2 Fate of mean field states and gauge theory

Now after performing the projective symmetry group analysis, we have a set of gauge-fixed mean field states. To study the stability of the mean field states, we include the gauge
fluctuation and ask when the fluctuation destroys the states. The question we are addressing is precisely the fate of the gauge fields coupled to the dynamical matter fields \[32, 35, 36\]. There have been many studies on this issue and we will just summarize some of those studies, which is relevant to our discussion.

The instability of the spin liquid we are mainly considering is the proliferation or condensation of the magnetic flux excitations such as a magnetic monopole in U(1) spin liquids or a vison in $\mathbb{Z}_2$ spin liquids. As the gauge field $a_\mu$ and the electric field $\vec{E}$ of $a_\mu$ are canonical conjugate to each other, it is energetically unfavorable for the electric field to stretch in the space if the magnetic fluxes are condensed. This effect is known as the dual Meissner effect. The spinon in the spin liquid carries the electric charge of $a_\mu$ and thus it is attached to the end of the electric flux. Hence the spinon, which is the source of the electric flux, ceases to exist as the force between two gauge charges are linear in distance between them. Hence the spinons will try to become a gauge neutral object, i.e., spin operator $\hat{S}_j$. In other words, the low energy physics where the magnetic excitation is condensed will be described solely by the spin operators and hence it does not have a fractionalization!

We call a phase which is obtained by condensing the magnetic excitations is called ‘confined phase’ \[37\], and the transition itself is called ‘confinement transition’. On the other hand the phase in which fractional excitations are free to propagate is called ‘deconfined phase’, and the spin liquid is a ‘deconfined phase’ of the associated gauge theory and the spinon is ‘deconfined’ in the spin liquid phase. One can ask if there is an order parameter for the confinement; at least for the pure gauge theory one can detect the confinement-deconfinement by looking at the Wilson loop operator \[37\] and how it behaves in its length e.g. if it increases as its perimeter (deconfined phase) or as its area (confined phase) of the loop.

With this information in hand, the natural questions are (1) when can or cannot a spin liquid be stable against the confinement? and (2) if there is a stable spin liquid, what will be the confined phase of the spin liquid? We are going to answer those questions subsequently.

**U(1) spin liquid**

In the U(1) spin liquid where the gauge field is always compact, the magnetic excitation driving a confinement transition is a magnetic monopole. In two dimension, the magnetic monopole is always proliferating \[36\] that there is no stable deconfined phase in the absence of the matter field in the low-energy theory. So if the mean field Hamiltonian \[1.39\] of the U(1) spin liquid has a gapped spectrum in two dimension, then the spin liquid state is unstable to the confinement and there is no such spin liquid state in reality. However if there are sufficiently many gapless matter fields, then there can be a stable deconfined phase \[38\]. With the gapped matter content, there is a way to get a stable deconfined phase. If the wavefunction of underlying matter fields is like a quantum Hall state, then it will support Chern-Simons theory in the gauge theory on top of the usual Maxwell theory \[1.41\]. This Chern-Simons theory will make the gauge photon, described by the Maxwell term, massive and spinon deconfined \[31, 32\]. In three dimension, there is a stable deconfined phase for the compact U(1) gauge theory for the gapped or gapless matter fields \[35\].
If the U(1) spin liquid becomes stable against the confinement, it always accompanies a gapless gauge photon as can be seen from (1.41).

$Z_2$ spin liquid

In the $Z_2$ spin liquid, the magnetic excitation driving a confinement transition is a $\pi$-flux, called a vison. The $Z_2$ gauge theories in two and three dimensions $^{[35]}$ have a stable deconfined phase for gapped or gapless matter contents. In two dimension, the vison is a particle-like excitation, but it is a loop excitation in three dimension.

Confined phase as symmetry broken phase

Though we may start from the stable deconfined phase, we can always access a confined phase of the gauge theory by tuning the fugacity of the magnetic excitations or some parameters in the Hamiltonian. We now address what phases we expect from the confinement transition.

As we embark from the spin liquid which does not break any symmetry, the symmetry-breaking patterns of the confined phase will be solely determined by the quantum numbers carried by the magnetic excitation to be condensed. There are many possibilities for the quantum numbers of the magnetic excitation, however usually the magnetic excitation is expected not to carry spin quantum number. Though there are some counter examples to this expectation, we concentrate on the case where the excitation is spinless.

As the spin liquid approaches the confinement transition, the fluctuation of the magnetic excitation will become larger and it starts to explore the dual lattice sites by hopping between the sites. On the other hand, there are huge electric flux emanating from the direct lattice site due to ‘a single spinon per site’ constraint $^{(1.36)}$, and this electric flux will modulate the motion of the magnetic excitations because there will be Berry phase for the magnetic excitation to move around the electric flux. For example, a vison in $Z_2$ spin liquid has mutually semionic statistics with the spinon and this implies that the vison will see the background of $\pi$ flux coming from a spinon sitting in a direct lattice site (which is equivalent to the dual plaquette). This means that the band structure of the magnetic excitation will be modulated, and this modulation will allow the minimum of the spectrum sitting other places than the center of the BZ. As like other bosons, the magnetic excitation will condense at the minimum of its spectrum and this means that the excitation will condense at the finite crystal momentum.

As the magnetic excitation does not carry the spin but the finite crystal momentum, the translational symmetry is broken but the spin rotational symmetry is intact in the confined phase. As the confined phase should be described only by the spin degrees of freedom, we look for a spin phase which is consistent with the broken translational symmetry and unbroken spin rotational symmetry: a valence bond solid phase. With more detailed analysis, one can usually make a precise connection between the confined phase and the valence bond solid phase.
However this is not all the lists of the confined phase and in the chapter 6 of this thesis we will show that there are interesting confined phases when the magnetic excitations are dressed with other quantum numbers by topological terms. On the other hand, in the chapter 7 it is of crucial issue that the magnetic monopole of the gauge field does not carry any other quantum number other than the crystal momentum.
Chapter 2

Overview of dissertation

The thesis is divided into three parts. In the first chapter, we establish topological field theoretic descriptions for the topological insulators and certain classes of $\mathbb{Z}_2$ spin liquids as the low-energy effective theory. We also demonstrate how the gapless edge theory can emerge from the pure topological field theory. The second chapter is devoted to the strongly interacting phases closely related to the topological insulators in the first chapter and their associate physics. We consider the confined phase of topological Mott insulator, a spin liquid with the topological band structure, and construct a bosonic symmetry protected topological insulator by utilizing a slave particle formalism developed in the introduction. In the last chapter, we illustrate that a topological Weyl semimetal can be realized by doping a conventional topological insulator material with magnetic materials and study its superconducting instability.

The first chapter consists of the three subchapters.

- “Topological BF field theoretic description of topological insulator”

  Topological phases of matter are described universally by topological field theories in the same way that symmetry-breaking phases of matter are described by Landau-Ginzburg field theories. We propose that topological insulators in two and three dimensions are described by a version of abelian $BF$ theory. For the two-dimensional topological insulator or quantum spin Hall state, this description is essentially equivalent to a pair of Chern-Simons theories, consistent with the realization of this phase as paired integer quantum Hall effect states. The $BF$ description can be motivated from the local excitations produced when a $\pi$ flux is threaded through this state. For the three-dimensional topological insulator, the $BF$ description is less obvious but quite versatile: it contains a gapless surface Dirac fermion when time-reversal-symmetry is preserved and yields “axion electrodynamics”, i.e., an electromagnetic $E \cdot B$ term, when time-reversal symmetry is broken and the surfaces are gapped. Just as changing the coefficients and charges of 2D Chern-Simons theory allows one to obtain fractional quantum Hall states starting from integer states, $BF$ theory could also describe (at a macroscopic level) fractional 3D topological insulators with fractional statistics of
point-like and line-like objects. This work has been published in *Annals of Physics, 326*, 1515, (2011) [39] and is done in collaboration with Joel E. Moore.

- **“Gapless edge states of BF field theory and translation-symmetric $Z_2$ spin liquid”**

  We study possible gapless edge states of translation-symmetric $Z_2$ spin liquids. The gapless edge states emerge from dangling Majorana fermions at the boundary. We construct a series of mean field Hamiltonians of $Z_2$ spin liquids on the square lattice; these models can be obtained by generalization of Wen’s exactly solvable plaquette model. We also study the details of the edge theory of these $Z_2$ spin liquids and find their effective BF theory descriptions. The effective BF theories are shown to describe the crystal momenta of the ground states and their degeneracies and to predict the edge theories of these $Z_2$ spin liquids. As a byproduct, we obtained a way to classify the BF theories reflecting the lattice symmetries. We discuss in closing three-dimensional $Z_2$ spin liquids with gapless surface states on the cubic lattice. This work has been published in *Physical Review B 86*, 125101 (2012) [40] and is done in collaboration with Yuan-Ming Lu and Joel E. Moore.

- **“Quantum phase transition and fractional excitations in a topological insulator thin film with Zeeman and excitonic masses.”**

  We study the zero-temperature phase diagram and fractional excitations when a thin film of 3D topological insulator has two competing masses: time-reversal symmetric exciton condensation and time-reversal symmetry breaking Zeeman effect. Two topologically distinct phases are identified: in one, the quasiparticles can be viewed as in a quantum spin Hall phase, and in the other a quantum anomalous Hall phase. The vortices of the exciton order parameter can carry fractional charge and statistics of electrons in both phases. When the system undergoes the quantum phase transition between these two phases, the charges, statistics and the number of fermionic zero mode of the excitonic vortices are also changed. We derive the effective field theory for vortices and external gauge field and present an explicit wave function for the fermionic zero mode localized at the excitonic vortices with or without orbital magnetic field. The quantum phase transition can be measured by optical Faraday or Kerr effect experiments, and in closing we discuss the conditions required to create the excitonic condensate. This work has been published in *Physical Review B, 84*, 165101 (2011) [41] and is done in collaboration with Joel E. Moore.

The second chapter consists of two subchapters.

- **“Dyon condensation in topological Mott insulators.”**

  We consider quantum phase transitions out of topological Mott insulators in which the ground state of the fractionalized excitations (fermionic spinons) is topologically non-trivial. The spinons in topological Mott insulators are coupled to an emergent compact $U(1)$ gauge field with a so-called “axion” term. We study the confinement transitions
from the topological Mott insulator to broken symmetry phases, which may occur via the condensation of dyons. Dyons carry both “electric” and “magnetic” charges, and arise naturally in this system because the monopoles of the emergent U(1) gauge theory acquires gauge charge due to the axion term. It is shown that the dyon condensate, in general, induces simultaneous current and bond orders. To demonstrate this, we study the confined phase of the topological Mott insulator on the cubic lattice. When the magnetic transition is driven by dyon condensation, we identify the bond order as valence bond solid order and the current order as scalar spin chirality order. Hence, the confined phase of the topological Mott insulator is an exotic phase where the scalar spin chirality and the valence bond order coexist and appear via a single transition. We discuss implications of our results for generic models of topological Mott insulators. This work has been published in New Journal of Physics, 14, 115030 (2012) [42] and is done in collaboration with Cenke Xu, Joel E. Moore and Yong Baek Kim.

• “Two dimensional symmetry protected topological phases with PSU(N) and time reversal symmetry.”

Symmetry protected topological phase is one type of nontrivial quantum disordered many-body state of matter. In this work we study one class of symmetry protected topological phases in two dimensional space, with both PSU(N) and time reversal symmetry. These states can be described by a SU(N) principal chiral model with a topological \( \Theta \)–term. As long as the time-reversal symmetry and PSU(N) symmetry are both preserved, the 1+1 dimensional boundary of this system must be either gapless or degenerate. We will also construct a lattice wave function of a spin-1 system on the honeycomb lattice, which is a candidate for the symmetry protected topological phase with both SO(3) and time-reversal symmetry. This work has been published in Physical Review B, 88, 014425 (2013) [43] and is done in collaboration with Jeremy Oon and Cenke Xu.

The third chapter again consists of two subchapters.

• “Possible topological phases of bulk magnetically doped Bi\(_2\)Se\(_3\): turning a topological band insulator into the Weyl semimetal.”

We discuss the possibility of realizing Weyl semimetal phase in magnetically doped topological band insulators. When the magnetic moments are ferromagnetically polarized, we show that there are three phases in the system upon the competition between topological mass and magnetic mass: topological band insulator phase, Weyl semimetal phase, and trivial phase. We explicitly derive the low energy theory of Weyl points from the general continuum Hamiltonian of topological insulators near the Dirac point, e.g. \( \mathbf{k} \cdot \mathbf{p} \) theory near \( \Gamma \) point for Bi\(_2\)Se\(_3\). We support the continuum calculation by studying the microscopic tight-binding model of magnetically doped topological insulator. This work has been uploaded online in arxiv:1110.1939 [27].
• “Superconductivity of doped Weyl semimetals: finite momentum pairing and electronic analogues of the $^3$He-A phase.”

We study superconducting states of doped inversion-symmetric Weyl semimetals. Specifically, we consider a lattice model realizing a Weyl semimetal with an inversion symmetry and study the superconducting instability in the presence of a short-ranged attractive interaction. With a phonon-mediated attractive interaction, we find two competing states: a fully gapped finite-momentum (FFLO) pairing state and a nodal even-parity pairing state. We show that, in a BCS-type approximation, the finite-momentum pairing state is energetically favored over the usual even-parity paired state and is robust against weak disorder. Though energetically unfavorable, the even-parity pairing state provides an electronic analogue of the $^3$He-A phase in that the nodes of the even-parity state carry non-trivial winding numbers and therefore support a surface flat band. We briefly discuss other possible superconducting states that may be realized in Weyl semimetals. This work has been published in Physical Review B, 86, 214514 (2012) [14] and is done in collaboration with Jens H. Bardarson, Yuan-Ming Lu, and Joel E. Moore.
Part I

Topological field theory descriptions of topological phases
Chapter 3

Topological $BF$ field theory
description of topological insulators

Most ordered phases of condensed matter can be classified using the concept of symmetry breaking, which leads to a theoretical description in terms of Landau-Ginzburg field theories. Such theories have had remarkable successes, such as the quantitative explanation of critical phenomena. Topological phases such as the quantum Hall effect require a different type of description in terms of “topological field theories”. These theories have the remarkable property that they are independent of the spacetime metric. The most famous example is the description of quantum Hall phases by Chern-Simons theory, which we review in a moment. As shown by Wen, that theory leads to detailed predictions about edge tunneling experiments on fractional quantum Hall samples, which to some degree have been verified at least qualitatively.

Recently new topological phases of electrons with time-reversal symmetry have been discovered. These “topological insulators” result from spin-orbit coupling and exist both in two and three dimensions, unlike the quantum Hall effect, which is essentially two-dimensional. These phases are insulating in bulk but support conducting edge or surface states. Hence one picture of a topological insulator is as a bulk insulator that necessarily has conducting edge or surface states; more recently there has been considerable interest in the electromagnetic response when a weak time-reversal-breaking perturbation gaps the surface state of the three-dimensional (3D) topological insulator. Our goal in this work is to find an effective field theory description of topological insulator phases in the same spirit as the Chern-Simons effective theory of the quantum Hall effect.

In order to understand why we do not consider the electromagnetic response in the 3D topological insulator to be a topological field theory in the sense of Chern-Simons theory, it is useful to review the quantum Hall case. In the quantum Hall effect, the Chern-Simons theory appears in two forms. We assume for now a single-component theory, such as describes the Laughlin states at $\nu = 1/k$. In terms of an internal gauge field $a_\mu$ and an integer $k$, the
Chern-Simons Lagrangian density is

\[ L_{CS} = \frac{k}{4\pi} \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda. \] (3.1)

Upon coupling this term to electromagnetic fields \( A_\mu \) by adding the term

\[ L_c = -J^\mu A_\mu, \quad J^\mu = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda} \partial_\nu a_\lambda. \] (3.2)

integrating out the internal gauge field \( a_\mu \) generates a term for the electromagnetic gauge field \( A_\mu \) that has the same Chern-Simons form as the internal gauge theory, but with coefficient \( \frac{k}{4\pi} \) rather than \( \frac{1}{4\pi} \). (Note that \( A_\mu \) does not include the background magnetic field generating the quantum Hall state.)

So for the quantum Hall effect, both the internal theory and the electromagnetic term have the same Chern-Simons form. The Chern-Simons theory on a closed two-dimensional manifold has a set of \( k^g \) zero-energy states, where \( g \) is the genus of the manifold, and an infinite gap to other states. The quantum Hall response is generated by the ground state’s response to electromagnetic perturbations in similar fashion to the superflow in a superconductor. On a manifold with boundary, the bulk Chern-Simons theory alone is not gauge-invariant, because under a gauge transformation, (3.1) changes by a total derivative. This total derivative leads to the topological part of the gapless edge theory; combining it with non-universal interactions from the edge gives the chiral Luttinger liquid description of edge states.

Our general goal is to carry through a similar program for topological insulators. We note that many features of three-dimensional topological insulators with gapped surfaces have been understood in terms of a total-derivative term for electromagnetic fields known as “axion electrodynamics” [13, 15]:

\[ L_{EM} = \frac{\theta e^2}{2\pi \hbar} \mathbf{E} \cdot \mathbf{B} = \frac{\theta e^2}{16\pi \hbar} \varepsilon^{\alpha\beta\gamma\delta} F_{\alpha\beta} F_{\gamma\delta}. \] (3.3)

This is analogous to the electromagnetic Chern-Simons term for \( A^\mu \) in the quantum Hall effect. It is “topological” in two senses: it is a total derivative of the electromagnetic Chern-Simons term, indicating that the surfaces where \( \theta \) changes support a half-integer quantum Hall effect. Its microscopic origin in a crystal is definitely topological as it involves the Chern-Simons form of the Berry connection of the Bloch electrons [13, 49–51].

We will argue that the natural description of the internal gauge theory takes a different form, which is one important difference between the quantum Hall and topological insulator cases. Note that one difference between the axion coupling (3.3) and the Chern-Simons term is that the axion term is gauge-invariant, while the Chern-Simons term is only gauge-invariant up to a boundary term. So any theory based purely on the axion coupling for an internal gauge field cannot generate a dynamical boundary from the requirement of gauge invariance in the way that the Chern-Simons theory does.
Section 3.1. Vortices with $\pi$ flux in a 2D topological insulator

Our approach leads to a version of $BF$ topological field theory in two and three dimensions as the effective description of topological insulators. This theory, which we introduce starting with the two-dimensional (2D) case in the following section, preserves time-reversal and parity symmetries, unlike the Chern-Simons theory; in particular it also can exist in three dimensions (3D), again unlike the Chern-Simons theory. In two dimensions, it is well known that the relevant $BF$ theory can be recast as two copies of Chern-Simons theory\[52, 53\], but we will argue that the $BF$ picture captures better the important properties of the 2D topological insulator, in particular its intrinsic time-reversal invariance.

We obtain the 2D $BF$ theory heuristically in the following section starting from the distinctive response of a 2D topological insulator to an electromagnetic $\pi$ flux (i.e., insertion of a solenoid with flux $hc/2e$)\[14, 54, 55\]. In 3D, the $BF$ theory involves one vector gauge field $a_\mu$ and one rank-two tensor field $b_{\mu\nu}$. These fields are associated with the distinctive response of a 3D topological insulator to a flux line\[56\], which is closely related to the response of the “weak” topological insulator to a dislocation\[57\]. So in both 2D and 3D we can understand $BF$ theory from the attachment of nontrivial responses to electromagnetic flux.

Section III introduces some general features of $BF$ theories of relevance to topological insulators, and Section IV provides more details for the 2D case. Section V contains most of the main results of this paper on the 3D case. One type of electromagnetic coupling is present even with time-reversal symmetry, while breaking time-reversal symmetry at the boundary is shown to lead to the $E \cdot B$ term after integrating out the internal fields of $BF$ theory. The electromagnetic current contains both “charge” and “polarization” contributions, and we obtain the “wormhole effect”\[56\] along flux lines with gapped surfaces as a consequence of the coupling. The existence of the Dirac fermion at surfaces when time-reversal-symmetry is present, which is the last result in Section V, becomes more understandable on noting that the combination of scalar and vector bosons that the bulk $BF$ theory implies at the surface are precisely those required to represent a Dirac fermion via the explicit “tomographic” mapping in 2+1D\[58, 59\].

Some generalizations and future directions are reviewed in Section VI; one is that the $BF$ theory description allows for fractional statistics not just in 2D but in 3D\[52, 53, 60, 61\]. This does not contradict the classic argument that pointlike objects do not have fractional statistics in 3D\[62\] because the fractional statistics are between one pointlike and one string-like object. As yet there is no microscopic realization of a “fractional” topological insulator (we discuss some issues in closing), but the $BF$ approach can at least formally describe such states. Rather than try to give an overview of the other features of $BF$ theory at the outset, it seems desirable to proceed with deriving it from the $\pi$ flux response in the simplest case, then explain how other features of topological insulators arise in the $BF$ theory.

3.1 Vortices with $\pi$ flux in a 2D topological insulator

In topological insulators, an electromagnetic $\pi$ flux has special roles both in 2D and 3D. When $\pi$ flux is threaded, there are always some excitations which are stable to any local $T$-
symmetric perturbation. In 2D TIs, π flux can induce spin-charge separation with semionic statistics. In 3D TIs, π flux creates helical 1D metals. Since this property is topological, π flux response can be used to distinguish TIs from trivial phases without referring to edge states. However, π flux is a strong perturbation from the point of view of an electron because the electron wavefunction gains a \((-1)\) phase factor when it is rotated around the flux. If our goal is to depict the TI as a condensed phase, as in the early work on the Chern-Simons description of the quantum Hall effect, then for the condensate to consist of charge \(e\) objects, the phase factor must be somehow compensated if the π flux is to be a finite-energy excitation.

So there must be another global effect that compensates the \((-1)\) phase factor for electrons when π flux is threaded. We will show that this is the origin of a BF-type action.

**Review of the 2π flux vortex**

Let’s consider a vortex threaded into a 2D condensate of charge \(e = 1\) objects (electrons). Consider the condensate wave function \(\psi\) and a \(U(1)\) electromagnetic gauge field \(A\) in a vortex configuration. The Lagrangian density for the single vortex follows \((\hbar = c = 1)\):

\[
L = \frac{1}{2} |(\partial_\mu - iA_\mu)\psi|^2 - V(\psi^\dagger\psi), \quad V = \frac{1}{2}(\psi^\dagger\psi - v^2)^2
\]  

The minimum energy configuration for \(\psi\) is easy to obtain: \(\psi = v \exp(i\theta)\) where \(\theta\) is the angle with respect to \(x\)-axis in 2D. This distribution of \(\psi\) has two key features. First, it minimizes the vortex potential \(V\). Second, \(\psi\) is single-valued because of the angle dependence \(\exp(i\theta)\). And if we substitute this distribution of \(\psi\) into equation (3.4), we obtain just

\[
L = \frac{v^2}{2}(\partial_\mu \theta - A_\mu)^2
\]  

The equation (3.5) fixes the field configuration of \(A\) to make the system have finite energy: \(A_i\) should be reduced into \(\partial_i \theta\) as \(r \to \infty\). Otherwise, the energy of the vortex is simply infinite which is not physically acceptable. Due to this constraint, the flux trapped in the vortex configuration is quantized by \(2\pi\):

\[
\int d^2x \varepsilon_{ij} \partial_i A_j = \oint d\vec{x} \cdot \vec{A} = \Delta \theta = 2\pi
\]  

In general, the single-valuedness requires \(\psi \propto \exp(in\theta)\) which corresponds to an \(n\)-vortex configuration. Then this gives the total flux \(2n\pi\) threaded in the 2D condensate. Hence, we directly see that π flux is not allowed for the vortex configuration with finite energy. Thus, we need another component in the theory to deal with π flux vortex.

**π flux vortex and BF theory**

As explained in the previous section, a finite-energy vortex configuration with π flux is seemingly excluded for a charge-\(e\) condensate. This result can be traced back to the
Section 3.1. Vortices with $\pi$ flux in a 2D topological insulator

phase factor $(-1)$ for electrons rotating around $\pi$ flux. Thus, if there is a way to create another phase factor $(-1)$ for electrons, then $(-1)(-1) = 1$ would allow $\pi$ flux in the vortex configuration with finite energy. This is done by introducing a $U(1)$ statistical gauge field $a_\mu$ that couples to electrons. This is depicted in the figure (3.1). Now the Lagrangian (3.4) is replaced by the following equation.

$$L = \frac{1}{2} |(\partial_\mu - i(A_\mu + a_\mu))\psi|^2 - V(\psi^\dagger \psi) \quad V = \frac{1}{2}(\psi^\dagger \psi - v^2)^2 \quad (3.7)$$

Both gauge fields $A$ and $a$ carry flux $\pi$ for the simplest case. However, $a$ can carry $(2n-1)\pi$ flux (or equivalently, $\pi$ flux of $a$ induces phase factor $\exp(i(2n-1)\pi) = (-1)$) because the single-valuedness of the wave function only requires the total phase change to be $2n\pi$ in rotating around vortex. For the purpose of deriving the BF-type action, $n = 1$ is enough, and we will stick to $n = 1$ in this section, but the generalization to $n \neq 1$ is trivial, and the importance for $n \neq 1$ will be pointed out later when we discuss the statistics of BF theory and the $\mathbb{Z}_2$-ness of TIs. With the same ansatz $\psi = v \exp(i\theta)$ as before, we get the Lagrangian density for the gauge fields $a$ and $A$:

$$L = \frac{v^2}{2}(\partial_\mu \theta - A_\mu - a_\mu)^2 \quad (3.8)$$

We can use the standard dual representation for the vortex by introducing an auxiliary $U(1)$ field $\xi^\mu$. Then the Lagrangian density (3.8) can be written as the following:

$$L = -\frac{1}{2v^2} \xi^\mu(\partial_\mu \theta - A_\mu - a_\mu) \quad (3.9)$$

Now the key step of the dual representation follows: writing $\theta = \theta_{\text{smooth}} + \theta_{\text{vor}}$. The integration (or gauging away) of $\theta_{\text{smooth}}$ gives the constraint $\partial_\mu \xi^\mu = 0$. This can be solved by introducing another $U(1)$ gauge field $b$ such that $\xi^\mu = \varepsilon^{\mu\nu\lambda}\partial_\nu b_\lambda$, and this transformation is enough to show there should be a BF-type term in the Lagrangian to deal with $\pi$ flux vortex. After using the relation between $\xi$ and $b$, we obtain

$$L = -\frac{1}{4v^2} f_{\mu\nu} f^{\mu\nu} + \varepsilon^{\mu\nu\lambda}\partial_\nu b_\lambda(\partial_\mu \theta_{\text{vor}} - A_\mu - a_\mu) \quad (3.10)$$

where $f$ is the field strength of $b$. Finally, we identify the vortex current as $j^\mu = \frac{1}{2\pi}\varepsilon^{\mu\nu\lambda}\partial_\nu \partial_\lambda \theta_{\text{vor}}$, and write the Lagrangian in a slightly different form:

$$L = -\frac{1}{4v^2} f_{\mu\nu} f^{\mu\nu} + 2\pi b_\mu j^\mu - \varepsilon^{\mu\nu\lambda}(A_\mu + a_\mu)\partial_\nu b_\lambda \quad (3.11)$$

Now we note that the first two terms in the equation (3.11) are induced by the vortex configuration, and argue that the effective theory for the background TI should be the third term including two gauge fields $a$ and $b$ with non-dynamical external gauge field $A$. Another
way to motivate discarding the first term is that, when we deal with long-range and low-
energy physics, we can ignore this Maxwell-like term for the same reason that pure Chern-
Simons theory is the effective theory for quantum hall systems: the third term in equation 
\[3.11\] includes only one derivative, whereas the Maxwell-like term carries two derivatives and 
is relatively small at long length scales. With slightly different normalization, we obtain the 
effective theory for the 2D topological insulator:

\[ L_{BF} = \frac{1}{\pi} \varepsilon^{\mu\nu\lambda}(A_\mu \partial_\nu b_\lambda + a_\mu \partial_\nu b_\lambda) \] (3.12)

The first term in equation \([3.12]\) is simply current-gauge coupling where the current is 
mediated by the gauge field \(b\). The second term is called the \(BF\) term (because it includes 
the gauge field \(b\) and the field strength of the \(a\) field), and it contains the coupling between \(a\) 
and \(b\). In fact, the \(BF\) term is topological, i.e it does not carry dynamics; rather it carries 
the information of statistics between sources of \(a\) and \(b\). The meaning of the coefficients and the 
\(BF\) term will be clarified in the next section, and in this section we focus on consequences 
of \([3.12]\). There is an interesting property for the equation \([3.12]\): if we integrate out \(a\) and \(b\), 
then the resulting action is 0, i.e., the bulk effective action for \(A\) is 0. So if we want to 
have an electromagnetic response due to the external gauge field \(A\), we need another term 
coupled to \(a\), as in the \(T\)-breaking Chern-Simons term for the quantum Hall effect. Another 
difference is that the \(BF\) theory with \(A\) above preserves \(P\)- and \(T\)- symmetry which will be 
clear in the next section. Looking ahead, a key feature of this \(BF\) theory is that it has a 
direct 3D generalization; for 3D, we will similarly derive the existence of a two-form gauge 
field \(b\) coupled to \(a\) and \(A\),

\[ L_{BF} = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho}(A_\mu \partial_\nu b_{\lambda\rho} + a_\mu \partial_\nu b_{\lambda\rho}) \] (3.13)

Then the equation \([3.13]\) inherits the properties of 2D \(BF\) theory \([3.12]\): it is topological, 
the effective action of \(A\) is zero, and it is \(P\)- and \(T\)- symmetric.

3.2 General properties of \(BF\) theory

Our goal in this paper is to argue that \(BF\) theory is the effective theory for TIs in a way 
similar to CS theory for the quantum Hall effect. Before continuing with that argument, 
let us review a few more properties of \(BF\) theory. \(BF\) theory is a generalization of CS 
theory, and both are topological \([52, 53, 63]\); in fact, the relationship between \(BF\) and CS 
theory is fairly simple in (2+1)D. This relationship is essentially the same as the microscopic 
relationship between (two copies of) the integer quantum Hall effect and the 2D TI. But there 
are important differences between \(BF\) and CS theory, such as symmetry; some similarities 
and differences between CS and \(BF\) theory in two and three spatial dimensions will be 
reviewed in the following. Versions of \(BF\) theory have been applied in condensed matter 
physics previously to study superconductors and topological spin liquids \([52, 63]\), but not
topological insulators as far as we are aware. Henceforth we follow the condensed matter convention and refer to systems by their spatial dimension, e.g., 2D means (2+1)D.

### 3.2.1 2D BF theory and CS theory

The most general form of BF theory in 2D is composed of two $U(1)$ gauge fields $a, b$ and corresponding sources $j, J$\cite{52, 53}. The full BF action is

$$L_{BF} = \frac{k}{2\pi} \epsilon^{\mu\nu\lambda} a_\mu \partial_\nu b_\lambda - j^\mu a_\mu - J^\mu b_\mu$$ \hspace{1cm} (3.14)

The first term in equation (3.14) is topological and describes braiding statistics with parameter $k$ : when the quasiparticle type $j$ is rotated around the quasiparticle type $J$, the total wave function obtains $\frac{2\pi}{k}$. This term has the same role as the term $L_{CS} = \frac{k}{4\pi} \epsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda$ in CS theory, and the equations of motion are also simply obtained:

$$\frac{k}{2\pi} \epsilon^{\mu\nu\lambda} \partial_\nu b_\lambda = j^\mu \hspace{1cm} \frac{k}{2\pi} \epsilon^{\mu\nu\lambda} \partial_\nu a_\lambda = J^\mu$$ \hspace{1cm} (3.15)

The symmetries of the gauge fields $a$ and $b$ are different: under $T$, $(a_0, a_1, a_2) \rightarrow (a_0, -a_1, -a_2)$ and $(b_0, b_1, b_2) \rightarrow (-b_0, b_1, b_2)$. So the BF term in the equation (3.13) is $T$- invariant. Armed with these, we reconsider the effective theory (3.12):

$$L_{BF} = \frac{1}{\pi} \epsilon^{\mu\nu\lambda} (A_\mu \partial_\nu b_\lambda + a_\mu \partial_\nu b_\lambda)$$ \hspace{1cm} (3.16)

Two comments about this theory are in order. First, because $(A_0, A_1, A_2) \rightarrow (A_0, -A_1, -A_2)$ under $T$- transformation (the same symmetries as the $a$ gauge field, which is why it is natural to describe the $\pi$ vortex by combining $A$ and $a$), we see that the theory is $T$- invariant, i.e., the minimal coupling between $A$ and $b$ is $T$- symmetric. $A$ acts as a source of $b$ field. Secondly, our theory for topological insulators is described by $k = 2$, and this makes sense because $\pi$ flux of $a$ field should give the phase factor $(-1)$ to the total wave function as we discussed $\pi$ flux vortex theory(\text{In fact, } k = 2 \text{ corresponds to the semionic statistics for } a \text{ and } b). However, this is not the only coefficient giving phase factor $(-1)$ between $a$ and $b$. In general, $k = \frac{2}{2n-1}$ should be equally good because $\exp(i(2n-1)\pi) = (-1)$. So the most general theory with $\pi$ flux having the proper statistical effect has the form :

$$L_{BF} = \frac{1}{(2n-1)\pi} \epsilon^{\mu\nu\lambda} a_\mu \partial_\nu b_\lambda + \frac{1}{\pi} \epsilon^{\mu\nu\lambda} A_\mu \partial_\nu b_\lambda$$ \hspace{1cm} (3.17)

For any value of $n$, the effective action for $A$ is still 0, so there is no (bulk) response to the external field $A$. Before getting into the details of the system’s response, it should be noted that the action of 2D BF theory is just doubled CS theory with opposite chirality; while it is known that the 2D TI can be realized as the double copy of quantum hall layers with opposite chirality, the above theory is saying that this is true for some properties, such as the
existence of edge modes, even when there is no conserved component of spin. The equation (3.12) can be equally well derived if we start from doubled CS theory and pick appropriate combinations of the two CS fields (“charge” and “spin”). However, it is well known that TIs can be described only by doubled CS theories describing odd-integer quantum Hall effects, and we wish to emphasize here that this is really coming from the $\pi$ flux response, which is a defining property of TIs, and not from the assumption of decoupled spin-up and spin-down layers.

3D $BF$ theory

The most general form of 3D $BF$ theory includes a one-form gauge field $a_\mu$, an antisymmetric two-form gauge field $b_{\mu\nu}$, and corresponding sources $j_\mu$, $\Sigma_{\mu\nu}$ [52, 53, 60, 61]. Here, the source $\Sigma$ is an antisymmetric rank 2 tensor, so physically the source $\Sigma$ represents the density of line-like objects that can be pictured as field lines for electric and magnetic parts of the tensor. We will later connect the magnetic and electric components of $\Sigma$ through the equations of motion. The corresponding $BF$ theory should contain information about braiding of vortices and quasiparticles. Interestingly, 3D $BF$ theory can be used to describe fractional statistics in 3D systems. The standard argument that pointlike particles cannot have fractional statistics in 3D as they do in 2D [62] is that all ways of looping one particle around another to detect their mutual statistics are topologically equivalent in 3D but not in 2D; as a result, 3D statistics are described by the permutation group, and 2D statistics are described by the much richer braid group—one consequence is that in 2D, there are “anyonic” particles that are neither fermionic nor bosonic. In 3D, vortices and quasiparticles can braid noncontractibly like particles in 2D, allowing for statistics other than fermionic and bosonic.

Hence it is possible to impose nontrivial statistics between vortices and quasiparticles, and we will argue that this is what happens in 3D TIs. The starting $BF$ theory is the following:

$$L_{BF} = k \frac{\epsilon^{\mu\nu\lambda\rho}}{4\pi} a_\mu \partial_\nu b_{\lambda\rho} - j_\mu a_\mu - \frac{1}{2} \Sigma_{\mu\nu} b_{\mu\nu}$$

(3.18)

As in the 2D case, the first term carries the statistics: when quasiparticle $j$ is rotated around the vortex density $\Sigma$, the total wave function obtains a phase factor $\frac{2\pi}{k}$. The equation of motion can be obtained by varying with respect to $a$ and $b$:

$$\frac{k}{4\pi} \epsilon^{\mu\nu\lambda\rho} \partial_\nu b_{\lambda\rho} = j_\mu \quad \frac{k}{2\pi} \epsilon^{\mu\nu\lambda\rho} \partial_\lambda a_\rho = \Sigma_{\mu\nu}$$

(3.19)

And as in 2D, $k = 2$ (or more generally, $k = \frac{2^n}{2n-1}$) will describe a TI for which threading with $\pi$ flux yields the correct phase factor $(-1)$. The external field $A$ acts as a source for the two-form field $b$ if we look into the equation [3.14]. Finally, this $BF$ theory is $T$-symmetric because $(a_0, a_1, a_2, a_3) \rightarrow (a_0, -a_1, -a_2, -a_3), (b_{0i}, b_{ij}) \rightarrow (-b_{0i}, b_{ij})$ and $(A_0, A_1, A_2, A_3) \rightarrow (A_0, -A_1, -A_2, -A_3)$. Thus the minimal coupling between $A$ and $b$ is still $T$-symmetric, and the candidate theory for 3D TIs with integer $n$ is following:

$$L_{BF} = \frac{1}{2(2n-1)\pi} \epsilon^{\mu\nu\lambda\rho} a_\mu \partial_\nu b_{\lambda\rho} + \frac{1}{2\pi} \epsilon^{\mu\nu\lambda\rho} A_\mu \partial_\nu b_{\lambda\rho}$$

(3.20)
As noted in 2D BF theory, we need a term coupled to $a$ to have a total bulk response of external gauge field $A$, which will be obtained later.

### 3.3 2D Topological Insulators

The physics of 2D TIs is relatively easy to understand compared to that of 3D TIs because a 2D TI can be realized as a bilayer integer quantum hall system with opposite $T$-symmetry, although this picture implicitly assumes a $U(1)$ spin rotation symmetry and fails to capture the $Z_2$ nature of the topological invariant. The role of the magnetic field in ordinary quantum hall systems is replaced by the spin-orbit interaction, whose symmetries require opposite integer quantum Hall states of up and down spins along the $U(1)$ axis.

#### 3.3.1 Quantum Hall Systems and CS theory

Let us consider a $\nu = \frac{1}{3}$ fractional quantum hall system, i.e., the lowest Landau level is $1/3$ full. The system has elementary excitations with fractional charges: fractionalized quasiholes($= \frac{e}{3}$) and quasi-electrons($= -\frac{e}{3}$). These excitations can be made in the system if we thread magnetic flux, and the braiding statistics of those quasiparticles are fractional. Remarkably, these seemingly complicated properties can be simply formulated in CS theory:

$$L_{CS} = -\frac{k}{4\pi} \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu a_\lambda + j^\mu a_\mu, \quad j^\mu = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda} \partial_\nu A_\lambda$$

(3.21)

Here $k$ parametrizes the braiding of quasiparticles and filling factor $\nu = \frac{1}{3}$ is described $k = 3$. The requirement of gauge invariance for the total action on a manifold with boundary, with $L_{CS}$ as bulk action, leads to an edge chiral boson field which is indeed present in quantum hall systems\[1, 64]. Moreover, if we integrate out the internal gauge field $a$, we obtain the correct effective electromagnetic Lagrangian for a state with Hall effect $\sigma_{xy} = e^2/3h$:

$$L_{QHE} = -\frac{1}{12\pi} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda$$

(3.22)

Thus we can argue that CS theory is a valid effective theory for quantum hall systems due to its correct description of statistics of quasiparticles, correct effective theory for $A$, and edge theory. In the next and subsequent sections, we will argue BF theory also captures statistics of quasiparticles, correct effective theory for $A$ and $B$, and edge theory of 2D TIs, i.e., BF theory should be the correct effective theory for TIs.

#### 3.3.2 2D Topological Insulators and BF theory

Topological insulators are gapped topologically ordered systems like quantum Hall states, and thus it is natural that they could be described by a topological field theory. However, BF theory, unlike the simplest form of CS theory, involves two entities in the theory $a$ and
Section 3.3. 2D Topological Insulators

b with different symmetries. If we want to follow the philosophy of CS theory, then a and b should couple to currents of elementary excitations in the system. So it would be good to think of possible excitations in TIs before moving into detailed mathematics.

To construct an analogy between CS theory and $BF$ theory, we will stick to 2D TIs in this section. In a quantum hall system, we can collect the elementary excitation by threading the magnetic flux. Similarly, we can thread a flux of the external electromagnetic gauge field into a 2D TI, and it is known that we can have two types of excitations in the presence of a $\pi$ flux[65]. In 2D TIs, the excitations are a charge-neutral Kramers doublet (charge 0 and, if one component of spin is a good quantum number, spin= $\pm \frac{1}{2}$) and holon(charge= $\pm e$ and spin zero). So a and b should couple to the sources of external gauge fields which are currents of “spinons” and “holons”; of course the external gauge field coupling to the Kramers-doublet is not physical, and the other gauge field is ordinary $U(1)$ electromagnetism.

Note that even if no $U(1)$ component of spin rotation symmetry like $S_z$ is conserved microscopically, there are still two $U(1)$ currents macroscopically, not just the $U(1)$ charge current. This is reflected in the existence of two dissipationless edge modes that are asymptotically decoupled at low energy, and the generic existence of a dissipationless “spin Hall effect” carried by edge states in an applied electric field even if the direction and magnitude of this spin Hall effect are not quantized. In the $BF$ description, there are two $U(1)$ currents of which one couples directly to the external electromagnetic field; the quantized particle source of the “spin” gauge field can be visualized as one of the charge-neutral excitations created by insertion of a $\pi$ flux.

We recall the previous $BF$ theory written for 2D TIs:

$$L_{BF} = \frac{1}{\pi} \varepsilon^{\mu \nu \lambda} (A_\mu \partial_\nu b_\lambda + a_\mu \partial_\nu b_\lambda)$$ (3.23)

From the above equation, we see that b couples to A and thus represents the field for holons. Naturally, a should represent spinons. More precisely, the current for a couples to a fictitious time-reversal gauge field $B$; the term for the coupling between spinons and external time-reversal gauge fields was absent in the the previous discussions because we only dealt with the physical EM field. To make the duality between a and b in 2D explicit, we now add $\frac{1}{\pi} \varepsilon^{\mu \nu \lambda} B_\mu \partial_\nu a_\lambda$ to our Lagrangian density. Then the full Lagrangian for our system is obtained:

$$L_{BF} = \frac{1}{\pi} \varepsilon^{\mu \nu \lambda} a_\mu \partial_\nu b_\lambda + \frac{1}{\pi} \varepsilon^{\mu \nu \lambda} A_\mu \partial_\nu b_\lambda + \frac{1}{\pi} \varepsilon^{\mu \nu \lambda} B_\mu \partial_\nu a_\lambda$$ (3.24)

The equations of motion for a and b can be obtained if we vary b and a.

$$\varepsilon^{\mu \nu \lambda} \partial_\nu b_\lambda = -\varepsilon^{\mu \nu \lambda} \partial_\nu B_\lambda, \quad \varepsilon^{\mu \nu \lambda} \partial_\nu a_\lambda = -\varepsilon^{\mu \nu \lambda} \partial_\nu A_\lambda$$ (3.25)

From the above equations, some important features can be directly read off. First, unit spinon and holon are localized at the $\pi$ flux of A and B from the equation of motion. Second, this spinon and holon obey semionic statistics. Thus, the above $BF$ theory (3.24) correctly describes the elementary excitations in 2D TIs. Now, consider the effective Lagrangian for
Figure 3.1: The black arrows represent one-half magnetic flux quantum (a $\pi$ flux) and the black spheres represent electrons. Consider a system with $S_z$ conservation for simplicity: an electron can be thought as a composite of a holon (red spheres) and an $S_z = \pm \frac{1}{2}$ spinon (blue spheres). a) Whenever an electron is circulated around the half flux quantum ($\pi$ flux), the electron acquires a phase factor ($-1$) which shifts the energy levels of electrons. b) This phase factor can be cured by introducing a statistical gauge field $a$ which is tied to the EM flux tubes; the $BF$ term does this job. Hence the electrons see an effective $2\pi$ flux and behave as though there is no flux tube present. c) Spinons and holons have relative semionic statistics and thus every holon is affected in the same way as an electron whenever there is a spinon present. This effect generates the phenomenon that EM $\pi$ flux captures one spinon and $\pi$ flux of the fictitious spin-gauge field captures one holon, as illustrated in d) and e).

By completing squares for $a$ and $b$ and integrating out them, we obtain the following effective Lagrangian:

$$L_{eff} = \frac{1}{\pi} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu B_\lambda$$

Note that there is no bulk electromagnetic action for $A$ alone, consistent with the absence of a charge Hall effect; the effective action for $A$ and $B$ in bulk describes a “quantum spin Hall effect” (a spin current flows in response to a charge field and vice versa) if there is a conserved current of spin in some direction. Since we can trivially rewrite the bulk $BF$ theory as a doubling of CS theory in 2D, it contains two chiral bosons at the edge, consistent with 2D TIs. We will review the derivation of this edge theory later in Section V as preparation for the surface theory of the 3D TI.

Before finishing this section, it is worth mentioning briefly how the $BF$ theory can capture the physics of the “$Z_2$ odd” property of 2D TIs. Consider an $N$-flavored $BF$ theory to
describe \( N \) copies of 2D TI

\[
L = \sum_{i=1}^{i=N} \left( \frac{1}{\pi} \epsilon^{\mu \nu \lambda} a^i_\mu \partial_\nu b^i_\lambda + \frac{1}{\pi} \epsilon^{\mu \nu \lambda} A^i_\mu \partial_\nu b^i_\lambda + \frac{1}{\pi} \epsilon^{\mu \nu \lambda} a^i_\mu \partial_\nu B_\lambda \right) \tag{3.27}
\]

This edge of this Lagrangian can be studied from the \( K \)-matrix of the system. The \( K \)-matrix for the single-flavor BF theory is \( K = \text{diag}(1, -1) \) when the BF term is diagonalized. This \( K \)-matrix captures that there are two one-dimensional edge modes with opposite chiralities. When there are \( N \) flavors, the \( K \)-matrix is trivially generalized as \( K = \text{diag}(1, -1, 1, -1, 1, -1 \cdots) \) where the block \( \text{diag}(1, -1) \) is repeated \( N \) times. This edge is unstable to \( T \)-symmetric perturbations if \( N \) is even. Thus, we are led to conclude \( N = (2n-1) \). This \( (2n-1) \)-flavor 2D TI can be fit into a single-component BF theory if we consider only the response to the external gauge fields. (That is, if we only look at the overall response to the external gauge fields, we do not actually need to retain the index \( i \) which labels different flavors, but can consolidate all flavors into one.) Then we are led to the simplified Lagrangian

\[
L = (2n-1) \times \left( \frac{1}{\pi} \epsilon^{\mu \nu \lambda} a_\mu \partial_\nu b_\lambda + \frac{1}{\pi} \epsilon^{\mu \nu \lambda} A_\mu \partial_\nu b_\lambda + \frac{1}{\pi} \epsilon^{\mu \nu \lambda} a_\mu \partial_\nu B_\lambda \right) \tag{3.28}
\]

This theory has a \( (2n-1) \)-times amplified spin Hall effect. This theory still has a well-defined response to the \( \pi \) fluxes as \( \pi \) flux is still the smallest \( T \)-symmetric flux. Hence, we still want to treat \( \pi \) fluxes as the unit sources of \( a \) and \( b \). This means we need to rescale the gauge fields \( a \) and \( b \): \((2n-1)a \rightarrow a \) and \((2n-1)b \rightarrow b \). This scaling applied to the Lagrangian (3.28) gives

\[
L = \frac{1}{(2n-1)\pi} \epsilon^{\mu \nu \lambda} a_\mu \partial_\nu b_\lambda + \frac{1}{\pi} \epsilon^{\mu \nu \lambda} A_\mu \partial_\nu b_\lambda + \frac{1}{\pi} \epsilon^{\mu \nu \lambda} a_\mu \partial_\nu B_\lambda \tag{3.29}
\]

which has been seen before when we considered \( \pi \)-flux responses.

In conclusion, BF theory can describe key aspects of 2D TIs: the importance of \( T \)-symmetry, the elementary excitations and their statistics, and the edge theory.

### 3.4 3D Topological Insulators

3D topological insulators are described by four \( \mathbb{Z}_2 \) topological invariants, one “strong” and three “weak”. Topological insulators with only nontrivial weak invariants can be adiabatically connected to layering of 2D topological insulators and are unstable to disorder. On the other hand, the strong topological insulator is an intrinsically 3D system and does not have a two-dimensional limit. Moreover, the essence of the 2D topological insulator can be understood relatively easily by considering “quantum spin Hall” systems where a \( U(1) \) subgroup of spin rotation symmetry is preserved. However, if we try to preserve a \( U(1) \) spin rotation in 3D topological insulators, we end up with only weak topological insulators rather than the strong topological insulator. This makes it difficult to understand the strong
topological insulator because we need information about spins in the system but we cannot identify states by a remaining spin quantum number.

BF theory supplies a route around this difficulty. Roughly speaking, the $b$ and $a$ fields in $BF$ theory carry information about spin and charge and couple to the external electromagnetic gauge field $A$. In this section, we will figure out what $a$ and $b$ should be on physical grounds and justify that our version of $BF$ theory is a correct effective description of 3D strong topological insulators: it captures the quantized magnetoelectric effect[13, 49] and the braiding of excitations in the system when the surfaces are gapped, and as mentioned in the Introduction it also allows the possibility of gapless fermionic surfaces.

### 3.4.1 3D topological insulators with gapped surfaces and $BF$ theory

As we did above for the 2D TI and $BF$ theory, we need to identify the coupling for the internal gauge field $a$. The $a$ field is still a one-form even in (3+1)D $BF$ theory, and the external gauge field $A$ is also a one-form. So the simplest coupling would be $\sim da \wedge dA$, but this breaks $T$- symmetry of the system as $T$ takes $da \wedge dA \rightarrow -(da \wedge dA)$. However, note that the term is a total derivative and hence can be sourced from a surface where its coefficient changes, i.e $da \wedge dA = d(a \wedge dA)$. Thus, we are led to conclude that our theory describes TI with broken $T$- invariance only on the surface. As before, we also have $T$- invariant couplings between $b$ and $a$, $A$. The resulting theory contains three terms.

\[
L_{BF} = \frac{1}{2\pi} \varepsilon^{\mu \nu \lambda \rho} a_\mu \partial_\nu b_\lambda b_\rho + \frac{1}{2\pi} \varepsilon^{\mu \nu \lambda \rho} A_\mu \partial_\nu b_\lambda \rho + C \varepsilon^{\mu \nu \lambda \rho} \partial_\mu a_\nu \partial_\lambda A_\rho \quad (3.30)
\]

We will find $Z_2$-ness, the existence of only two phases as a result of $T$ invariance, by studying the third term in the theory. To proceed further, we need an extra piece of information which is not encoded in the field theory itself: the gauge charge lattice. This is because the response to EM field is sensitive to the quantization of charges in the system. For convenience, we deal with a compact (3+1)D manifold such as $T^4$. On such manifolds, we have no boundary and hence the third term might be thought to be trivial. However, this is not the case as we will consider $T$- invariance of the theory. We separate the terms in the theory $[3.30]$ as follows: $L_{\text{bulk}} = \frac{1}{2\pi} \varepsilon a \partial b + \frac{1}{2\pi} \varepsilon A \partial b$ and $L_{\text{surf}} = C \varepsilon \partial a \partial A$ where anti-symmetrization is done implicitly. The full theory is $\exp(i \int (L_{\text{bulk}} + L_{\text{surf}}))$. Under the time-reversal symmetry operation, we obtain $\exp(i \int (L_{\text{bulk}} - L_{\text{surf}}))$. Hence, for the theory to be well-defined and have $T$- symmetry, we need to have $\exp(i \int L_{\text{surf}}) = \pm 1$.

Now, we impose the gauge charge lattice for the theory. First, there is a well-defined particle excitation $j^a_0$ which is the source for the gauge $a$. We quantize $j^0_a$ to be integral over each of the 2D tori within $T^4$. Then from the second term in $L_{\text{bulk}}$, we are led to conclude that $j^0_{em}$ is also quantized to be an integral multiple of $e$. This seemingly trivial imposition of the gauge charge lattice gives a nontrivial effect on $L_{\text{surf}}$ as the fluxes threaded in each ‘torus’ of the manifold should be quantized by $\frac{2\pi}{e} = 2\pi$ (here $e = 1$ in our units). Then $L_{\text{surf}}$
can take only the following possible values.

\[
\int L_{\text{surf}} = C 2\pi Z \times 2\pi Z \times 2 = C 8\pi^2 Z. \tag{3.31}
\]

Here \(Z\) indicates an unknown integer. The first \(2\pi Z\) is due to the integral of \(\partial A\) and the second \(2\pi\) is due to the equation of motion connecting \(\partial a\) to \(\partial A\). In result, we conclude that \(\exp(i \int L_{\text{surf}}) = \pm 1\) as \(C = 0, \frac{1}{8\pi} \text{mod} \frac{1}{4\pi}\), and the topologically non-trivial insulator corresponds to \(C = \pm \frac{1}{8\pi}\).

Now, we integrate out \(a\) and \(b\) fields in the equation (3.30) with \(C = \frac{1}{8\pi}\) so that we get the magnetoelectric effect of the strong topological insulator\[13\],

\[
S_{3D} = \pm \int d^3x dt \frac{1}{8\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\mu A_\nu \partial_\lambda A_\rho \tag{3.32}
\]

Now we introduce the theta-angle \(\theta = C \times 8\pi\) which is the usual “axion electrodynamics”\[15\] of the topological insulator. Because of the quantization of \(C\), we have \(\theta \sim \theta + 2\pi\). We allow \(d\theta \neq 0\) on the surface of the topological insulator, which then influences the rest of the material through the \(\partial a \partial A\) term.

With this knowledge and the full Lagrangian, we can now study other properties of the system by the equations of motion resulting from equation (3.30). Before getting into the details of the equations of motion for \(a\) and \(b\), it is important to notice that electromagnetic current is conveyed by both \(a\) and \(b\). The current can be directly read off from the equation (3.30) by \(\delta L_{BF}/\delta A\).

\[
J_{EM}^\mu = J_b^\mu + J_a^\mu = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\nu b_\lambda \rho + \frac{1}{8\pi^2} \varepsilon^{\mu\nu\lambda\rho} \partial_\nu (\theta \partial_\lambda a_\rho) \tag{3.33}
\]

So the total electromagnetic current is carried by both gauge fields \(a\) and \(b\). Even though the two terms of this current appear similar, the interpretation of \(a\) and \(b\) will show that the two are independent contribution to \(J_{EM}\).

It is easy to interpret the contribution from \(b\) : \(b\) is a two-form and thus can be thought of as related to ordinary particle current in the same way as the field strength in electromagnetism. Because \(J_b\) is a free-particle current in the TIs, we might expect \(J_b\) to appear only on the edge as the Hall current when we solve the equation of motion for \(b\), and it turns out to be so. For \(J_a\), we need to be somewhat careful. The term including \(J_a\) is originally from the surface \(L_{\text{surf}}\). Here we treat the term as a part of bulk theory. Thus, if we only ask about the bulk current, \(J_a = 0\) trivially. But \(J_a\) need not be zero on the surface. Actually, \(J_a = \hat{n} \cdot P + \hat{n} \times M\) where \(P\) is electric polarization, \(M\) is magnetic polarization and \(\hat{n}\) is the normal vector to the normal. To see this, we revisit \(L_{\text{surf}}\) for the case \(\theta = \pi\):

\[
L_{\text{surf}} = \frac{1}{8\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\mu a_\nu \partial_\lambda A_\rho = \frac{1}{2} F^{\mu\nu} \partial_\mu A_\nu = \frac{1}{2}( \vec{P} \cdot \vec{E} + \vec{M} \cdot \vec{B} ) \tag{3.34}
\]
Here $P^{\mu\nu}$ is the antisymmetric polarization tensor, $\vec{P}, \vec{M}$ are usual electric, magnetic moments. We identify $\vec{P}_i = P^0_i$ and $\vec{M}^i = P^{jk}_i$ where $P^{\mu\nu} = \frac{1}{4\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\lambda a_\rho$. The polarization has an additional constraint like usual polarization in neutral matter: $\partial_\nu P^{\mu\nu} = 0$ implying that $\nabla \cdot \vec{P} = 0$ and $\nabla \times \vec{M} = 0$. From this constraint, we can see that we split the electromagnetic response into two pieces that cannot mix up. One part is $J_a$ which is particle-like response, and the second part is $P^{\mu\nu}$ which is like string or polarization response. With these in mind, we can cast our $BF$ theory into the physically straightforward form

$$L_{BF} = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} a_\mu \partial_\nu b_\lambda A_\rho + J_0^i b_i + \frac{1}{2} (\vec{P} \cdot \vec{E} + \vec{M} \cdot \vec{B})$$

(3.35)

The second term is the usual coupling of the EM field and charge current. The third term is the coupling allowed by symmetry between (magnetic and electric) polarizations and the EM field. The term shows up only in the nontrivial topological insulator. Finally, the first term gives nontrivial braiding between particle and polarizations. This description will give in the next section the axion electrodynamics form of EM responses of topological insulators with gapped surfaces that break $T$-symmetry once we integrate out the $a$ and $b$ fields. If on the other hand we did not break $T$-symmetry on the surfaces, then we will obtain a different description as seen below.

Before finishing this section, we present the equations of motion for the fields $a$ and $b$ for future use. We vary $a$ and $b$ for the Lagrangian (3.30). The resulting equations are as follows:

$$\frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\nu b_\lambda A_\rho = \pm \frac{1}{8\pi^2} \varepsilon^{\mu\nu\lambda\rho} \partial_\nu \partial_\lambda A_\rho, \quad \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\lambda A_\rho = -\frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} \partial_\lambda A_\rho$$

(3.36)

Given $A$, we can obtain part of $a$ and $b$ according to these equations of motion. Effectively, $A$ is the source for $a$ and $b$. The most studied example for 3D TI is an EM flux tube threading the bulk and its surface. The gauge configuration for $a$ is easy to capture as it describes another vortex tied to EM vortex with the same magnitude. On the other hand, we need to be careful for $b$ as $b$ has more gauge degrees of freedom. For convenience, we think of a TI with $z < 0$ and the magnetic flux threading the surface at the origin. We stick to the static configuration of $A$ fields. Then the equation for the gauge $b$ can be split into two parts:

$$J_0^i = \frac{1}{8\pi} \delta(x) \delta(y) \delta(z), \quad \frac{1}{2\pi} \partial_i \varepsilon^{ijk} b_{jk}, \quad J_b^i = 0 = \frac{1}{2\pi} (\nabla \times b^0)^i,$$

(3.37)

where we used $\partial_0 b = 0$ for the second equation. These two equations imply that the end of the flux tube is a monopole source for $\varepsilon b_{jk}$, and $b^0$ has a curl-free configuration. This is illustrated in Fig. 3.2.

### 3.4.2 Gapped Edge Theory of 3D Topological Insulators

In this section, we will establish the “edge theory” of the surface of a 3D TI once time-reversal-breaking perturbations have been added. (We use edge theory in this section for
Figure 3.2: A flux tube threads a 3D TI and penetrates the surface. a) The black arrow represents the magnetic flux and the black sphere represents the localized EM charge due to the QHE on the surface. The equations of motion for $a_\mu$ and $b_{\mu\nu}$ give the distribution of the gauge fields. b) The picture for $a_\mu$ is simple: the $a_\mu$ gauge field generates another flux tube at the location of the $A$ flux tube. The tensor gauge field $b_{\mu\nu}$ can be broken up into two pieces $b^{0i}$ and $\epsilon_{ijk}b^{jk}$. With the flux configuration of $A$, c) $b^{0i}$ sees a monopole source at the surface and d) $\epsilon_{ijk}b^{jk}$ sees no source but should be curl-free according to the equation of motion. The picture of $b_{\mu\nu}$ is determined only up to the gauge freedom of the field, which consists of adding any divergence-free vector field for $b^{0i}$ and adding any curl-free vector field for $\epsilon_{ijk}b^{jk}$.

comparison to the well-known edge theories of 2D topological states. That the surface in our $BF$ theory should be $T$-broken is visible in $L_{surf}$.) Generically the surface is gapped for $T$-symmetry-breaking perturbations present on the surface. The gapped surface should not change the bulk properties much for weak perturbations, and we expect the edge theory to reflect some properties of the bulk theory. In fact, 3D $BF$ theory generates the topological term of 2D $BF$ theory as its edge theory, plus additional terms reflecting the broken time-reversal symmetry. The edge 2D $BF$ theory inherits topological properties from 3D bulk $BF$ theory. In this section, we derive the gapped edge theory of 3D TI in the same way as CS theory predicts a gapless edge theory of quantum Hall states, and we explore the properties of the theory including the effects of an infinitely thin flux tube threading a 3D TIs.
Review of the edge theory of CS theory

In this section, we briefly review the derivation of the edge theory for CS theory in 2D. For simplicity, we ignore the coefficients and confine ourselves to understanding the requirements imposed by the gauge invariance of the theory. We follow Wen’s argument leading to the edge theory of fractional quantum Hall states from gauge invariance of the theory on a manifold with boundary [1]. Let us denote the compact bulk as $M$ and the boundary as $\partial M$. The bulk action for CS theory is $S_0 = \int_M a \wedge da$ which is not gauge invariant. For a general gauge transformation $a \rightarrow a + d\gamma$, the action changes $S_0 \rightarrow S_0 - \int_{\partial M} d\gamma \wedge a$.

Hence we introduce a scalar field $\phi$ living on the edge and gauge transform $\phi \rightarrow \phi + \gamma$ when $a \rightarrow a + d\gamma$. Now gauge invariance forces us to write the action for our system as $S = S_0 - \int_{\partial M} d\phi \wedge a$. However, the Hamiltonian related to $\int_{\partial M} d\phi \wedge a$ is zero. So we need an extra term to get the usual chiral edge theory; this term reflects physics localized near the edge, while the zero-energy Hamiltonian reflects a topological kinetic energy part coming from the bulk.

To introduce the edge term, we define the covariant derivative $D\phi = d\phi - a$, which is gauge invariant under any gauge transformation, and we write the Lagrangian $S = S_0 - \int_{\partial M} d\phi \wedge a - C \int_{\partial M} D\phi \wedge * (D\phi)$ where $*$ is the dual operation. The key points in deriving the edge theory can be summarized as: 1) we can restore gauge invariance by introducing fields at the edge, and 2) the term $D\phi \wedge * (D\phi)$ is not coming from the gauge invariance of the bulk theory, but rather is an extra piece required for the theory to have non-trivial dynamics at the edge. This surface dependence is manifest in that the coefficient for this term in the edge chiral theory depends on the material; it determines the propagation velocity of the edge excitations. Now we use similar arguments to derive the edge theory of 3D $BF$ theory.

Gapped Edge theory of 3D $BF$ theory

In this section, we derive the edge theory [66] of 3D $BF$ theory by requiring the total theory with surface to have the same gauge invariance as the interior of the 3D sample. While doing so, another important feature of the bulk $BF$ term shows up; the bulk $BF$ theory is not gauge invariant, just as above for CS theory. The surplus gauge degree of freedom goes to the edge and establishes the edge theory. We will initially study the case when the surface is gapped by a time-reversal-breaking perturbation, then return in the last part of this chapter to the question of how massless fermions appear when time-reversal symmetry is present.

As before, we ignore the numerical coefficients at first but will restore the coefficients later as the coefficients determine the statistics and Hall effect on the edge. We start with the edge theory without external EM gauge field $A$. The answer for this system can be written simply by introducing a new scalar field $\Phi$ whose values only are significant on the boundary and writing $a' = a + d\Phi$:

$$S = \int_M b \wedge da' - \int_{\partial M} b \wedge a' .$$

(3.38)
This combined action is explicitly gauge-invariant if we define \( \Phi \) to transform \( \Phi \rightarrow \Phi - \gamma \) when \( a \rightarrow a + d\gamma \). (Note: \( \Phi \) describes degrees of freedom only on the edge since in the bulk term \( da = da' \).) It is elementary to check the gauge invariance when \( b \rightarrow b + d\xi \). (We do not allow the variation with respect to \( b \) on the edge; rather we vary \( a \) and \( \Phi \) independently.) When we vary the nondynamical field \( \Phi \) to obtain a constraint, we have \( db = 0 \), i.e., \( b \) is pure gauge on the edge. Thus \( b = d\zeta \) at least locally for the 2D edge by Poincare’s Lemma and the edge action becomes simply 2D BF theory \( \int_{\partial M} a \wedge d\zeta \).

When we include the coupling to an external gauge field \( A \), still the same idea applies and thus we can derive the edge theory. If we add \( b \wedge dA \) and \( \theta da \wedge dA \) to the bulk action, then the term \( b \wedge dA \) requires a term \( b \wedge A \) on the edge. However, \( \theta da \wedge dA \) is itself gauge invariant, so we do not need any additional term in the edge action and we can move the term \( \theta da \wedge dA = d(\theta a \wedge dA) \) freely to the edge for the case \( d\theta = 0 \) in the bulk, or vice versa.

So we write the action for \( M + \partial M \) as

\[
S = \int_M (b \wedge da' + b \wedge dA + \theta da \wedge dA) - \int_{\partial M} (b \wedge a' + b \wedge A - \theta da \wedge dA) \tag{3.39}
\]

We can move the term \( \theta da \wedge dA \) into the edge by Gauss’s Law:

\[
S = \int_M (b \wedge da' + b \wedge dA) - \int_{\partial M} (b \wedge a' + b \wedge A - \theta da \wedge dA) \tag{3.40}
\]

The two actions \( (3.39) \) and \( (3.40) \) are physically equivalent. If we integrate out \( a \) and \( b \) in equation \( (3.39) \), then we obtain \( S \sim \int_M \theta dA \wedge dA \). On the other hand, if we integrate out \( a \) and \( b \) in equation \( (3.40) \), we obtain \( S \sim \int_{\partial M} A \wedge dA \), identical to the case of equation \( (3.39) \). This illustrates that we can move every physical response to the EM gauge field to the edge by moving the term \( \theta da \wedge dA \). The effect of pushing this term to the edge is not only a surface Hall effect but also statistical, and we will discuss this effect again later. For later use we restore the important coefficients for the action now. We take the edge to lie in the \( xy \) plane and assume that \( b \) is the pure gauge \( d\zeta \) on the edge. Then

\[
S = \int_M \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} b_{\mu\nu} \partial_\lambda a_\rho + \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} b_{\mu\nu} \partial_\lambda A_\rho + \frac{\theta}{8\pi^2} \varepsilon^{\mu\nu\lambda\rho} \partial_\mu a_\nu \partial_\lambda A_\rho - \int_{\partial M} \frac{1}{\pi} \varepsilon^{\mu\nu\rho} \zeta_\mu \partial_\nu a_\rho + \frac{1}{\pi} \varepsilon^{\mu\nu\rho} \zeta_\mu \partial_\nu A_\rho \tag{3.41}
\]

Some comments are worthwhile here. First, the gauge invariance of the theory is guaranteed by \( \zeta_\mu \rightarrow \zeta_\mu + \xi_\mu \) when \( b_{\mu\nu} \rightarrow b_{\mu\nu} + \partial_\mu \xi_\nu - \partial_\nu \xi_\mu \), and the gauge transformation of \( a \) leaves the theory invariant as \( a \) appears only as \( d \wedge a \).

Secondly, when we move the term \( \theta da \wedge dA \) into the edge as \( \theta a \wedge dA \), \( \theta \) term appearing in the edge action should be interpreted as \( d\theta = \theta_{TI} - \theta_{vacuum} \), and \( \theta \) itself is not well-defined on the edge so the term proportional to \( da \wedge dA \) is breaking \( T \) symmetry. Lastly, the sources of \( b \) in bulk and \( \zeta \) on the surface are the same. If there is a source \( \tau \) of \( \zeta \) on the surface that enters as \( \tau^\mu \zeta_\mu \), then \( \tau \) should be a part of \( \Sigma_{\mu\nu} \) threading the surface (explicitly, \( \tau^0 = \hat{n}_i \cdot \Sigma^{0i} \).
where \( \hat{n} \) is the normal vector to the surface. Thus, there is no local excitation at the surface for \( b \) or \( \zeta \) fields. With the full machinery, we take the edge action of the 3D bulk action as the following:

\[
S_{\text{edge}} = \int_{\partial M} \left( \frac{1}{\pi} \varepsilon^{\mu\nu\rho} \zeta_\mu \partial_\nu a_\rho + \frac{1}{\pi} \varepsilon^{\mu\nu\rho} \zeta_\mu \partial_\nu A_\rho + \frac{\theta}{8\pi^2} \varepsilon^{\mu\nu\rho} a_\mu \partial_\nu A_\rho \right) \tag{3.42}
\]

For the bulk action of equation (3.42), we have

\[
S = \int_M \left( \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} b_{\mu\nu} \partial_\lambda a_\rho + \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} b_{\mu\nu} \partial_\lambda A_\rho \right), \tag{3.43}
\]

which is trivial for the \( A \) field when \( a \) and \( b \) are integrated out: in this form the entire electromagnetic response comes from the surface.

**Infinitely Thin Flux Tube**

In this section, we calculate the charge bound to a flux tube by using the gapped edge action we derived in the previous section. This provides some intuition for the meaning of the fields in the effective theory. We thread a \( \pi \) flux tube through the 3D TI adiabatically. The flux tube is inserted into a thin cylinder in 3D TIs, and the surface of the cylinder is itself an edge of the 3D TI. While doing so, we will use the gapped edge action because the cylinder is also part of the edge and thus gapped (i.e., we assume the same \( T \)-breaking perturbation continues along the cylinder). Unfortunately, we cannot get the gapless edge theory discussed in the next section from the gapped edge action by naively plugging in a \( \pi \) flux configuration of \( A \) field, but we can glimpse the effects of degrees of freedom living in the \( \pi \) flux tube of 3D TIs.

From the action for edge (3.42), there can be at most two degrees of freedom carried by \( \zeta \) and \( a \). Thus, we can guess there are possibly two chiral modes to the gapless cylinder surface because of time reversal properties (or no localized mode); indeed there are two gapless chiral modes at the infinitely thin cylinder with \( \pi \) flux as expected. Now, we calculate the charge bound to the \( \pi \) flux at the end of the flux tube. For simplicity, we imagine an infinite bulk with the cylindrical hole at the center and assume that the flux remains spatially separated from the surface of the cylinder. We take the \( x \)-axis along the cylinder axis and the \( y \)-axis around the cylinder on the surface (We compactify \( y \) direction). Thus, the flux \( \Phi \) threaded in the cylinder is given by the integral of \( A_y \) along the \( y \) direction.

\[
\Phi(t) = \int A_y(t) dy \tag{3.44}
\]

Given this external field \( A \), we have equations of motion for \( \zeta \) and \( a \). Before deriving the equations of motion, we first identify the EM current due to external EM gauge field by \( \frac{\delta}{\delta A} S \) where \( S \) is the action for the edge:

\[
J^\mu_{\text{EM}} = j^\mu_\zeta + j^\mu_a = \frac{1}{\pi} \varepsilon^{\mu\nu\rho} \partial_\nu \zeta_\rho + \frac{1}{8\pi} \varepsilon^{\mu\nu\rho} \partial_\nu a_\rho \tag{3.45}
\]
where we plugged $\theta = \pi$. The equations of motion for $\zeta$ and $a$ are easily derived by varying with respect to $a$ and $\zeta$.

$$j^\mu_\zeta = \frac{1}{8\pi} \varepsilon^{\mu\nu\rho} \partial_\nu A_\rho, \quad j^\mu_a = \frac{1}{8\pi} \varepsilon^{\mu\nu\rho} \partial_\nu A_\rho$$

Thus, we have the following equation for the total current flowed along the cylinder.

$$Q = \int dt J_{EM}^x = \int dt dy \frac{1}{4\pi} \partial_t A_y = \frac{\Phi}{4\pi}$$

Because the total flux at the end of threading process is $\pi$, we obtain charge $\frac{e}{4}$ localized at the one side end of the flux tube and $-\frac{e}{4}$ on the other side end of the flux. We wish to emphasize that this localized charge is exactly what is expected from the surface hall effect. When the surface of the TI is gapped, the surface hosts $\frac{1}{8\pi}$ (half the conductance quantum; $e = \hbar = 1$) Hall conductance, and thus we have charge $\frac{e}{4}$ when $\pi$ flux is threaded. One more comment is in order: as the surface explicitly breaks $T$- invariance, we can deduce that the system distinguishes $\pi$ from $-\pi$ as far as the flux threads the surface. A consequence is that the charge localized at the tip of $\pi$ flux is different from that of the $-\pi$ flux. However, if the flux totally lies in the bulk by making it a torus, then the system never distinguishes $\pi$ flux from $-\pi$ flux. This can be easily seen from the bulk Lagrangian.

$$L = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} a_\mu \partial_\nu b_\lambda b_\rho + \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda\rho} A_\mu \partial_\nu b_\lambda b_\rho$$

From this Lagrangian, we see that $\pi$ flux is one unit of vorticity of the $b$ gauge field. Upon encircling a unit source of $a$ around the $\pi$ flux, the wave function obtains a phase factor $\exp(i\pi)$ which is equivalent to $\exp(-i\pi)$ where $-\pi$ flux is in place of $\pi$ flux. Having reproduced the expected properties for gapped surfaces, we now turn to the emergence of Dirac fermions at the surface of $BF$ theory when time reversal is unbroken.

**Gapless Edge Theory of 3D $BF$ theory**

Rather than a problem, it is a useful feature of 3D $BF$ theory that the bulk theory by itself is not invariant under gauge transformations on a manifold with boundary. The gauge fields forced to live at the edge cancel out the surplus gauge freedom of the bulk theory. Here we will study the gapless surface of 3D $BF$ theory and will find explicit expressions for a surface Dirac fermion field, constructed from the bosonic fields topologically required to exist at the surface of a 3D topological insulator. Combined with the ability to reproduce the expected electromagnetic coupling for gapped surfaces, this fermionic boundary suggests strongly that 3D $BF$ theory is the proper topological field theory for the 3D strong topological insulator.

The basic idea is that 3D $BF$ theory contains two bosonic fields at the edge[52], one arising from $a_\mu$ and the other from $b_{\mu\nu}$. From these two bosonic fields, it is not obvious at first sight how to construct a fermion. Fortunately, there are bosonized theories for (2+1)D fermions (and other higher dimensions as well[69]) which were originally constructed to generalize the
well-known bosonization of (1+1)D fermionic systems. The key idea of these constructions, which can be made precise in terms of the “topographic” representation\[58, 59\], lies in describing the higher-dimensional system as an infinite number of (1+1) dimensional 'rays'. The complicated part is in maintaining the Fermi statistics of particles belonging to different rays. We will find that the Dirac fermion constructed out of the two bosons predicted by \(BF\) theory shows the special property of the surface of 3D topological insulators that the momentum and the spin of electrons are locked to each other.

In this section, we first start with the edges of 2D \(BF\) theory to clarify the structure of the surface edges of 3D \(BF\) theory, and move into the surface of 3D \(BF\) to obtain a Dirac fermion. While we are dealing with the surface of 3D \(BF\) theory, we show that there are two gapless bosonic fields on the surface of 3D \(BF\) theory and proceed to the "tomographic" transformation of introducing rays. We can then compare the result to the bosonization of a single Dirac fermion.

In order to emphasize the similarities between the 2D and 3D TIs in the \(BF\) description, we review the edge of the 2D \(BF\) theory first and see how the surface theory of 3D \(BF\) can be thought of as an infinite number of “rays” described by the edge theory of 2D \(BF\) theory.

To get the edge theory of 2D \(BF\) theory, we start by solving the bulk equations of motion of the 2D bulk \(BF\) theory, i.e \(a_k = \partial_k \Lambda\), and \(b_k = \partial_k \Gamma\) with Coulomb gauge \(a_0 = b_0 = 0\). Up to a constant,

\[
\int_M L = \int_M \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu b_\lambda = \int_{\partial M} (\partial_t \Gamma)(\partial_x \Lambda) + (\partial_x \Gamma)(\partial_t \Lambda)
\]

where \(M\) is 2D bulk, and the dynamics on its edge \(\partial M\) is described by the fluctuations of \(\Lambda\) and \(\Gamma\). We see that there is a first-order edge Lagrangian from the bulk: the Hamiltonian is zero until we add additional non-universal terms generated by the boundary.

The physics becomes more transparent if we take symmetric and antisymmetric combinations of \(\Lambda\) and \(\Gamma\). Substituting \(S = (\Lambda + \Gamma)/2\) and \(A = (\Lambda - \Gamma)/2\) into the equation (3.49),

\[
\int_{\partial M} (\partial_t \Gamma)(\partial_x \Lambda) + (\partial_x \Gamma)(\partial_t \Lambda) = \int_{\partial M} (\partial_t S)(\partial_x S) - (\partial_x A)(\partial_t A)
\]

The surface is assumed to generate the term

\[
H = \int \frac{v_1}{2} (\partial_x A)^2 + \frac{v_2}{2} (\partial_x S)^2
\]

Where \(v_1\) and \(v_2\) are the speeds of fluids and is system dependent. We identify the fluid density operators \(\rho_1(x) = \partial_x S\) and \(\rho_2(x) = \partial_x A\). The equations of motions for \(A\) and \(S\) are now understood as the continuity equations for the fluids,

\[
\partial_t \rho_i(x, t) + (-1)^i v \partial_x \rho_i(x, t) = 0, \quad i = 1, 2
\]

Thus, there are two chiral bosonic modes flowing in opposite directions. Moreover, we can see that the spectrum of the Hamiltonian (3.51) is \(v|k|\) after quantization where \(|k|\) is the magnitude of the one-dimensional momentum, and time-reversal symmetry forces \(v_1 = v_2\).
These bosonic modes can be viewed as the density excitations of a one-dimensional fermionic system via standard 1+1-dimensional bosonization.

We now wish to follow the same general prescription for the surface of 3D $BF$ theory: we obtain bosonic fields and a kinetic term from the bulk action and add potential terms assumed to arise from non-universal physics at the surface. The result is then shown to be a bosonized version of a 2+1-dimensional free Dirac fermion satisfying the expected conditions for a TI surface. Starting with the $BF$ theory with no $T$-breaking surface term and solving the bulk equations of motions for $a$ and $b$ with Coulomb gauge ($a_i = \partial_i \Lambda, b_{ij} = \partial_i \zeta_j, \text{ and } a_0 = b_0 = 0$), we obtain (up to an overall constant)

$$\int_M L = \int_{\partial M} \partial_t \Lambda \varepsilon^{ij} \partial_i \zeta_j + \partial_t \Lambda \varepsilon^{ij} \partial_i \zeta_j$$

(3.53)

Hence the surface theory contains a scalar field $\Lambda$ and a vector field $\zeta$, from which we need to construct fermions. The same surface theory for 3D $BF$ theory has been obtained previously\[52\]; we are not aware that the following connection between $BF$ theory and surface Dirac fermions or topological insulators has been made before. The topological part of the surface action for $BF$ theories more generally is discussed in Appendix B of Reference\[70\].

We assume that the effect of non-universal surface physics is to generate the potential terms

$$H = \int (\alpha_1 (\partial_t \Lambda)^2 + \alpha_2 (\varepsilon^{ij} \partial_i \zeta_j)^2)$$

(3.54)

analogous to the potential terms at the quantum Hall edge. The constants $\alpha_1$ and $\alpha_2$ are non-universal and will ultimately determine the velocities of excitations, which we assume to be isotropic; henceforth we set $\alpha_1 = \alpha_2 = 1$ so that the velocities of propagation are unity and we can connect to some previous field theory literature. The surface equation of motion from varying $\Lambda$ is

$$\partial_t \varepsilon^{ij} \partial_i \zeta_j - \nabla^2 \Lambda = 0$$

(3.55)

which is the total derivative of

$$\partial_t \varepsilon^{ij} \zeta_j - \partial_t \Lambda = 0.$$  

(3.56)

The equation of motion from varying $\zeta_i$ is similarly the total derivative of

$$\partial_i \Lambda - \partial_t \varepsilon^{ij} \zeta_j = 0.$$  

(3.57)

But (3.56) and (3.57) are precisely the “Bose structure” on one scalar and one vector boson that are required to construct massless fermionic fields via the tomographic representation; the key equation (21) of Reference\[58\] is just the above with $B \to \Lambda, A \to \zeta$, and we switch to that paper’s notation in the following. For self-containedness and to make this result less mysterious, we reproduce the key steps from that work and the explicit expression for the Dirac spinors. Note that the first-order kinetic energy term obtained from $BF$ theory is not what would be obtained from, e.g., fluctuations of an elastic surface; a bosonization approach to the TI surface seemingly inequivalent to ours has recently been proposed by Vildanov\[71\] starting from a modified hydrodynamics of an incompressible fluid.
We now proceed to the tomographic representation for the scalar $A$ and vector $B$, and we will quantize them to obtain two bosonic fields describing two incompressible fluids. The tomographic representation uses the following generalized delta function:

$$\delta^{1/2}(y - \hat{n} \cdot r) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk |k|^{1/2} e^{iky} e^{-ik\hat{n} \cdot r} = \frac{1}{2\pi} \int_0^\infty dk k^{1/2} \cos k(y - \hat{n} \cdot r)$$  \hspace{1cm} (3.58)

This function is used to transform the usual cartesian representations of fields into the tomographic representation. For example, the tomographic transformation of a scalar field $\phi(r)$ is defined as

$$\tilde{\phi}(y, \hat{n}) = \int dr \delta(y - \hat{n} \cdot r) \phi(r).$$  \hspace{1cm} (3.59)

Physically, $y \in (-\infty, \infty)$ represents the projected distance of $r$ from the origin along the direction $\hat{n}$. From now on, we write $\theta$ for the direction of $\hat{n}$, i.e. $\hat{n} = (\cos(\theta), \sin(\theta))$. Scalar, spinor, and vector fields in the tomographic coordinates are denoted with an extra tilde.

From this definition, the following two useful relations can be obtained:

$$\delta(r - r') = \frac{1}{4\pi} \int dyd\theta \delta(y - \hat{n} \cdot r) \delta(y - \hat{n} \cdot r'),$$  \hspace{1cm} (3.60)

$$\frac{1}{2\pi} \int d^2r \delta(y - \hat{n} \cdot r) \delta(y' - \hat{n}' \cdot r) = \delta(y, y') \delta(n, n') + \delta(y, -y') \delta(n, -n').$$  \hspace{1cm} (3.61)

Note that the second equation manifests the connection between $(\hat{n}, y)$ and $(-\hat{n}, -y)$ that appears below in the identification of the surface theory as a single Dirac fermion in condensed matter language. These are the standard tools for the tomographic representations of bosonization theory\cite{58, 59, 72}.

With the radiation gauge for $A$ ($\nabla \cdot A = 0$), after tomographic transformation of $A$ and $B$ one obtains\cite{58}

$$\partial_\theta \tilde{B}(y, \hat{n}) = \partial^\tau_\theta \tilde{A}(y, \hat{n})$$

$$\partial_y \tilde{B}(y, \hat{n}) = \partial^\tau_0 \tilde{A}(y, \hat{n}),$$  \hspace{1cm} (3.62)

and the longitudinal part of $\tilde{A}$ is constant and can be ignored. These describe bosons propagating with nonzero velocity along each ray direction $\hat{n}$. A spinor field in tomographic coordinates can be constructed for each ray as a normal-ordered version of

$$\tilde{\psi}(y, \hat{n}) = C \exp(i\sqrt{\pi} \left[ \tilde{A}(y, \hat{n}) + \tilde{B}(y, \hat{n}) \right]),$$  \hspace{1cm} (3.63)

where $C$ is a normalization constant. The last step is to add a 2D “Klein factor” that ensures the canonical anticommutation relations of fermions are satisfied not just on one ray but between different rays; the end result is that $\tilde{\psi}$ is multiplied by an operator\cite{58}

$$O_{\hat{n}} = \exp \left( \frac{i\sqrt{\pi}}{2} \int_0^\theta d\theta' \left[ \alpha(\hat{n}(\theta')) + \beta(\hat{n}(\theta')) \right] \right)$$  \hspace{1cm} (3.64)
where the charges $\alpha$ and $\beta$ are

$$
\alpha(\hat{n}) = \int_{-\infty}^{\infty} \partial_0 \tilde{A}(y, \hat{n}) \\
\beta(\hat{n}) = \int_{-\infty}^{\infty} \partial_0 \tilde{B}(y, \hat{n}) .
$$

This fermion propagates with unit velocity in the $+y$ direction and is the tomographic transform of a 2D massless Dirac fermion. A subtle point is that there is another fermion field $\tilde{\chi}$ propagating in the $-y$ direction, but we note that the Hermitian conjugate of $\tilde{\chi}(-y, -\hat{n})$ is equivalent to $\tilde{\psi}(y, \hat{n})$ up to a phase factor and conclude that the above indeed describes just one fermion propagating in each direction; note that the surface-dependent chemical potential needs to be specified to determine the relative excitation energies of “electron” and “hole” propagating in a given direction.

Hence the physical picture of the gapless edge of $BF$ theory is as follows. The scalar and vector boson fields have a kinetic term from the bulk theory and a potential term from the surface theory, as in the Chern-Simons case. These combine to allow the faithful representation of Fermi fields. The details of the surface determine both the velocities on each ray and the filling of the Fermi states, i.e., the chemical potential. It is well understood that the remarkable power of bosonization for interacting systems in one dimension does not carry through straightforwardly to higher dimensions, essentially because the ray decomposition of the Hilbert space (a “superselection rule”) is less useful for normal interactions. The $BF$ theory of topological insulators predicts that interactions in the bulk still lead to massless Dirac fermions via the bulk-edge connection derived in this section, and additional interactions occurring at the surface can be more naturally treated in the emergent fermionic variables than the bosonic ones. A future direction that we comment on briefly below is to consider the surfaces of fractional topological insulators in three dimensions.

### 3.5 Conclusions and future directions

We have argued that a topological field theory of $BF$ type is the effective theory of 2D and 3D topological insulators. For the 2D topological insulator, this can be understood easily when one direction of spin is conserved and the system separates precisely into two copies of the quantum Hall effect. The $BF$ description of the 3D topological insulator is our main result; perhaps the most surprising property is the emergence of surface Dirac fermions from the particular kinetic term of scalar and vector bosonic fields that are forced to exist by the incomplete gauge invariance of $BF$ theory.

There are several obvious generalizations and future directions that can be pursued. Considerable recent interest has gone into classifying topological insulators and superconductors with other symmetries than time-reversal, including their responses with gapped surfaces, which are the analogues of the $\mathbf{E} \cdot \mathbf{B}$ response in the conventional topological insulator. Such systems may also be described by topological field theories, and it would be interesting
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Figure 3.3: a) Illustration of the tomographic representation of a distribution $P = P(x,y)$, which is depicted as the red object. The tomographic projection is to project the distribution on the line along $\hat{n}$ and is described as the blue dashed density on the line spanned by $\hat{n}$. b) and c) explain why $(\hat{n}, y)$ is the same as $(−\hat{n}, −y)$, as a projection onto $(\hat{n}, y)$ is equivalent to the projection onto $(−\hat{n}, −y)$.

to find the appropriate theories for those systems and the field-theory description of their defects and interfaces.

We will focus in closing on one particular direction where we believe $BF$ theory holds considerable promise. Consider the Chern-Simons effective theory of the integer quantum Hall effect. Multiplying the coefficient of the Chern-Simons term by 3 immediately gives the essential features of the fractional quantum Hall effect state previously described microscopically by Laughlin, including the braiding statistics and modified scaling dimension of the electron operator at the edge, which can be probed in tunneling experiments.

In the same way, we can obtain an effective theory for potential fractional 3D topological insulators by modifying the coefficient of the $BF$ term. It should be stated from the outset that there is not yet a microscopic parent Hamiltonian for a 3D fractional topological insulator. Recent constructions of effective descriptions of 3D fractional topological insulators have been based on “parton” ideas: the electron fractionalizes into a combination of other particles, one of which (a neutral spinon\footnote{16} or a fractionally charged object\footnote{16, 17}) then forms a topological insulator state. The $BF$ theory presented here leads to a picture of 3D fractional topological insulators that appears somewhat different. Changing the coefficient of the braiding term to another of the set of possible values\footnote{16} leads to fractional statistics between point-like and line-like objects. For a single pair of fields $(a_\mu, b_{\mu\nu})$, gapped surfaces will have surface quantum Hall layers of Hall conductance $1/2, 1/6, 1/10, \ldots$, where the first
is the “integer” topological insulator studied in this paper and all surface Hall conductances are ambiguous by an integer.

The most interesting aspect of such a fractional topological insulator might be its gapless surface theory. Each 1D ray in the tomographic representation is now a pair of chiral Luttinger liquids with renormalized scaling dimension of the electron operator, i.e., essentially the effective theory discussed previously \cite{18} for the edge of a 2D fractional topological insulator. The 2D surface state formed from the collection of such rays would be an unusual non-Fermi-liquid state worthy of future study. Leaving this fractional case aside, we can conclude from the results in this paper that $BF$ theory can describe the universal physics of the currently extant topological insulators just as Chern-Simons theory captures the universal physics of quantum Hall states.

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Chapter 4

Gapless edge states of BF field theory and translation-symmetric Z2 spin liquid

The recent discovery of a classification\textsuperscript{[20, 79–81]} for various topological insulators and superconductors\textsuperscript{[45, 82, 83]} relies on discrete symmetries of the non-interacting fermions. For example, band insulators respecting time-reversal symmetry can be classified in two and three spatial dimensions. In both cases there are two distinct classes of band insulators which cannot be smoothly connected to each other. For the non-trivial phase of time-reversal symmetric insulators in three dimensions\textsuperscript{[6–8]}, gapless states of Dirac fermions emerge on its surface. The gaplessness is protected as long as the time-reversal symmetry is respected at the boundary and the bulk gap remains finite.

This is very different from the physics of the fractional quantum Hall effect (FQHE)\textsuperscript{[3, 84]}, which is one of the most well-understood and rich examples of topological order\textsuperscript{[2, 85]}. On the edge of a fractional quantum Hall state, there is a gapless chiral Luttinger liquid\textsuperscript{[86, 87]} which can never be gapped out simply because the net chirality of the bulk state prevents some modes from disappearing. There is no reference to symmetry needed to explain the stability of the edge states in FQHE. Moreover, the topological order of the FQHE is intimately connected to the gapless edge state\textsuperscript{[88]}. The connection between the topological bulk theory and the edge theory is easily understood from effective Chern-Simon theory\textsuperscript{[2, 88]} of the FQHE. In this effective theory description, the edge degree of freedom is encoded in the gauge invariance of the Chern-Simons theory with an open boundary.

However, Z2 spin liquids, which are also one of the well-established examples of topological order, do not have gapless edge states in general. The effective $BF$ theory\textsuperscript{[52, 89, 90]} description of Z2 spin liquid does have an edge degree of freedom as in the Chern-Simons theory: the edge theory is a pair of chiral fermions propagating in opposite directions. In the absence of any symmetry, these two fermion modes can backscatter to open up a gap\textsuperscript{[52, 89]} in contrast to the “chiral” Chern-Simons theory of FQHEs. This is true as far as no symmetry is imposed and can be generalized to any ‘doubled’ theory\textsuperscript{[91]}. However, it is known that
the edge theory of the Abelian ‘doubled’ theory can be gapless when $U(1)$-charge conservation and time-reversal symmetry are present. The physical example of this is the fractional (and integer) quantum spin Hall effect. As an Abelian ‘doubled’ theory can be re-written formally as the $BF$ theory (at the level of the Lagrangian) and a $Z_2$ spin liquid is described by $BF$ theory, one might think that the edge theory of $Z_2$ spin liquids can be also gapless if the time-reversal symmetry is imposed. This is, in fact, incorrect for $Z_2$ spin liquids.

The reason why $Z_2$ spin liquids fail to have a gapless edge state is traced back to the differences in the charge lattice of the compact gauge theory (or equivalently, the differences in the allowed operators of the edge theory due to quantization). We will see that the $Z_2$ conservation of charge and vortices in $Z_2$ spin liquids is crucial. We will expose this ‘structural’ difference of the formally identical theories in the subsequent discussion in this paper. Nonetheless, the understanding of the gapless edge states of the fractional spin Hall effect indicates that the doubled theories can have gapless edge states. Thus, it implies that $Z_2$ spin liquids will have gapless edge states if the correct symmetries are imposed on top of the topological order. In this paper, we will show that translational symmetry can stabilize the gaplessness of $Z_2$ spin liquids in certain cases. We make a direct connection between the microscopic structure of the physics and the effective $BF$ theory to confirm the gaplessness of the edge states.

Another motivation of this paper is to study the effect of the translational symmetry on the so-called “intrinsic topological order”. The intrinsic topological orders in gapped phases are featured by long-range entanglement, fractional excitations, and topological degeneracies. Examples of intrinsic topological orders are the fractional quantum Hall effect states and gapped quantum spin liquids. Intrinsic topological orders are stable against any weak perturbations in the presence of no symmetry, to compare with “symmetry-protected topological order”. The symmetry-protected topological (SPT) phases include topological insulators and topological superconductors as its outstanding examples. One SPT phase is a gapped phase with no fractional excitations and no topological degeneracy, which has gapless boundary states protected by symmetry. Most importantly, a gapped SPT phase can be continuously connected to the trivial phase if the symmetry is broken. A natural question is: what kind of role does symmetry play for intrinsic topological orders? It turns out that different symmetry enriched topological (SRT) phases can emerge from the same intrinsic topological order, such as different classes of fractional topological insulators with $U(1) \times Z_2^T$ symmetry. Therefore fractional topological insulators and other SRT phases exhibit interesting interplay of fractionalization and symmetry. Here, we show that by imposing translational symmetry new physics emerges in $Z_2$ spin liquids such as gapless edge states and the Majorana zero modes at the lattice dislocations.

The rest of the paper is organized as follows. In section 4.1 we will study the general edge theory of $Z_2$ spin liquids and show that the edge theory is generally gapped when there is no symmetry imposed on top of the $Z_2$ topological order. We also compare the edge theory of $Z_2$ spin liquids to the edge theory of the quantum spin Hall insulator. In section
III, we impose translational symmetry on Z2 spin liquids. We reveal the structure of Wen’s plaquette model, which has a gapless edge state, and generalize it to construct mean field Hamiltonian of Z2 spin liquids with gapless edge states. We also study the edge theory in detail, including the condition for the existence of the gapless edge states and its stability. In section IV, we encode the lattice translational symmetry into the $BF$ theory and make a connection between $BF$ theories and the Z2 spin liquids found in section III. We present a generalization to a three-dimensional model in section V, then summarize our results and raise open questions in section VI.

### 4.1 General Discussion of edge theory of Z2 spin liquids

In Z2 spin liquids, there are two low-energy excitations, namely the spinon and the vison. Spinons (visons) carry electric charge $e = 1$ (magnetic charge $m = 1$) in the underlying $Z_2$ gauge theory. They can be described by $BF$ theory with the charge lattice $e \in Z_2$ and $m \in Z_2$. We denote the electric current $J_\mu$ and magnetic current $j_\mu$ which couple to $a_\mu$ and $b_\mu$ minimally. Then, the low-energy theory for the $Z_2$ spin liquid\cite{52, 89, 90} is

$$L = \frac{1}{\pi} \varepsilon^{\mu\nu\lambda} a_\mu \partial_\nu b_\lambda - a_\mu J_\mu - b_\mu j_\mu + O(\partial a, \partial b)^2. \quad (4.1)$$

As noted before, a formally similar $BF$ theory emerges as the effective theory for the spin Hall effect with a Kramer pair of counter-propagating gapless edge modes. To manifest this similarity, we diagonalize the $BF$ Lagrangian into two copies of Chern-Simon theory, i.e., we write $A_\mu = a_\mu + b_\mu$ and $B_\mu = a_\mu - b_\mu$ to obtain

$$L = \frac{1}{4\pi} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda - \frac{1}{4\pi} \varepsilon^{\mu\nu\lambda} B_\mu \partial_\nu B_\lambda - A \cdot \chi - B \cdot \tau, \quad (4.2)$$

where the dot product $(A \cdot J = A_\mu J^\mu)$ are understood. We introduced the source currents $\chi = \frac{J + j}{2}$ and $\tau = \frac{J - j}{2}$ for $A_\mu$ and $B_\mu$. The charge lattice associated with $\chi$ and $\tau$ can be deduced from that of $J$ and $j$ (i.e., of $e$ and $m$). We begin with $(e, m = 0)$ where $e$ is defined modular 2. For $e = 0$ and $m = 0$, $(\chi, \tau) = (0, 0)$. For $e = 1$ and $m = 0$, $(\chi, \tau) = (1/2, 1/2)$. For $e = 2 \sim 0 \text{ mod } 2$ and $m = 0$, $(\chi, \tau) = (1, 1) \sim (0, 0)$. Similar consideration shows that $(\chi, \tau) = (1, -1) \sim (0, 0)$. Thus, in the diagonalized doubled Chern-Simon theory, $(\chi, \tau) = (1, \pm 1) \sim (0, 0)$ is the same as $(e, m) = (2, \pm 2) \sim (0, 0)$ in $BF$ theory. Now, we construct the edge theory from Eq.\(4.2\).

$$L_{\text{edge}} = \psi_R^\dagger (\partial_t - v \partial_x) \psi_R + \psi_L^\dagger (\partial_t + v \partial_x) \psi_L \quad (4.3)$$

This edge theory, in general, is unstable to opening up a gap\cite{52, 89}. This can be easily seen from $Z_2$ conservation of spinons and visons. The $Z_2$ gauge charge conservation allows us to add the mass term $\sim \psi_R^\dagger \psi_L, \psi_L^\dagger \psi_R$ and $\psi_R \psi_L, \psi_R^\dagger \psi_L^\dagger$. This is because $\psi_R^\dagger \psi_L, \psi_L^\dagger \psi_R$, or
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\[ \psi_R \psi_L, \psi_R^\dagger \psi_L^\dagger \] carry charges \((\chi, \tau) = (1, \pm 1)\) which are equivalent to no charge \((\chi, \tau) = (0, 0)\) in \(Z_2\) theory. Hence, we conclude that there is no protected edge state for a general Z2 spin liquid without additional symmetries, independent of microscopic constructions. However, this could be changed when the Z2 spin liquid is supplemented by a symmetry. Additional symmetries on the topological order can restrict the form of the mass terms and stabilize the gapless edge state.

We now show that the time-reversal symmetry cannot stabilize the ‘gaplessness’ of the edge states of Z2 spin liquids (if it does not possess any ‘strong index’ \([6]\) for the underlying fermionic spinons). We take the edge theory Eq.(4.3) and consider the time-reversal symmetry operation on the \(A_\mu\) and \(B_\mu\). Due to the fact that under time reversal \(T : A_\mu \rightarrow (-1)^\mu B_\mu\) and \(B_\mu \rightarrow (-1)^\mu A_\mu\) (with the definition \((-1)^\mu = 1\) for \(\mu = 0\) and \((-1)^\mu = -1\) for \(\mu = 1, 2\)) under the time-reversal operation, the time-reversal operation effectively acts as the exchange of two fermionic fields, i.e., \(T : \psi_R \rightarrow \psi_L\) and \(\psi_L \rightarrow e^{i\theta} \psi_R\) up to the \(U(1)\) phase factor \(e^{i\theta}\). We can take \(\theta = \pi\) or 0 to be consistent with the time-reversal operation \(T^2 = (-1)^N_f\) or \(T^2 = 1\), where \(N_f\) represents the total fermion number operator. This operation should be supplemented with \(v \rightarrow -v\). Hence, the kinetic term for the edge theory Eq.(4.3) is time-reversal symmetric. We discuss the two different cases \(T^2 = 1\) and \(T^2 = (-1)^N_f\) independently. First, for \(T^2 = 1\) the time-reversal symmetry allows mass terms of the form \(\psi_R^\dagger \psi_L\), with an equal amplitude for \(\psi_L^\dagger \psi_R\), which are capable of gapping the edge. Other terms such as \(\psi_R \psi_L\) are not allowed. As a whole, the time reversal symmetric edge theory for Z2 spin liquid is

\[
L = L_{\text{edge}}(\psi_R, \psi_L) + m(\psi_R^\dagger \psi_L + \psi_L^\dagger \psi_R) + h.c., \tag{4.4}
\]

where \(L_{\text{edge}}\) is the kinetic term Eq.(4.3). For \(T^2 = (-1)^N_f\), \(\psi_R^\dagger \psi_L\) and \(\psi_L^\dagger \psi_R\) are not allowed. Instead, there are allowed terms such as \(\psi_R \psi_L\), and they are enough to gap out the edge state. Here we assumed that there are no strong indices for the underlying spinons. The strong index includes the \(Z_2\)-indices for DIII class and \(Z\) indices for C/D classes \([20, 79]\) for band structures of the Schwinger fermions \([107, 112]\) (fermionic spinons). When the strong index of the time-reversal symmetry is nontrivial, then this phase automatically has the gapless edge state which is either a pair of helical Majorana modes (DIII class) or chiral Majorana modes (C or D classes). However, these phases are not described by BF theory \([1]\) and will not be discussed in this work.

For the quantum spin Hall effect on the other hand, we have \(U(1)\) charge conservation and the time-reversal symmetry \(T\) with \(T^2 = (-1)^N_f\). The two conditions exclude \([92]\) the two mass terms \(\psi_R^\dagger \psi_L, \psi_R \psi_L\) which were allowed in \(Z_2\) theory. Hence, the edge excitations of the quantum spin Hall state are gapless, in contrast to that of Z2 spin liquids.

\(\text{If the Schwinger fermion band structure lies in Class C, it corresponds to a chiral spin liquid whose effective theory is a } U(1) \text{ Chern-Simons theory. In the case of class D and DIII, the corresponding spin liquids host non-Abelian quasiparticle excitations which could in general be described by non-Abelian Chern-Simons theory.}\)
In the remaining sections of this paper, we will consider the effects of the translational symmetries on the states localized at the edges of $Z_2$ spin liquids. We find that translational symmetry can stabilize the gapless modes at the edges of some $Z_2$ spin liquids.

### 4.2 Wen’s plaquette model and mean field theory of $Z_2$ spin liquids

Wen’s plaquette model\footnote{113} is an exactly solvable model on the square lattice where the spin degrees of freedom are fractionalized into Majorana fermions. The model can be formulated as the pure $Z_2$ gauge theory\footnote{114}

$$H = -g \sum_P F_P = -g \sum_P \prod_{<ij> \in P} U_{ij}, \quad (4.5)$$

where $P$ denotes a plaquette of the direct lattice. Here, $U_{ij} = \pm 1$ is the $Z_2$ gauge field on the link $< ij >$, and thus $\prod_{<ij> \in P} U_{ij} = F_P$ is the field strength on the plaquette $P$. A faithful representation of this gauge theory is $U_{i,i+\hat{x}} = i\lambda_{i,x} \chi_{i,x}$, $U_{i,i+\hat{y}} = i\lambda_{i,y} \chi_{i,y}$ with translational symmetry. There are four Majorana fermions ($\lambda_{i,x}, \chi_{i,x}, \lambda_{i,y}, \chi_{i,y}$) per site, and the dimension of the Hilbert space per site is $2^4 = 4$ states per site (see Fig.4.1). To faithfully represent a spin-1/2 system, we need to halve this Hilbert space, i.e., the Hilbert space per site should have dimension 2. This is done by taking the $Z_2$ redundancy into account: the theory Eq.(4.5) is invariant under $U_{ij} \rightarrow s_i U_{ij} s_j$, $s_i = \pm 1$. The model can be more clearly represented if we introduce two complex fermions

$$f_{i,u} = \lambda_{i,x} + i\chi_{i,x}, \quad f_{i,d} = \lambda_{i,y} + i\chi_{i,y}, \quad (4.6)$$

such that the spin $\vec{S}_i$ on the site $i$ is represented via $\frac{1}{2} \sum_{\alpha,\beta} f_{i,\alpha}^\dagger \sigma^{\alpha,\beta} f_{i,\beta}$. Then, the Hamiltonian Eq.(4.5) reduces to

$$H = -g \sum_P S_{i,x} S_{i+\hat{x},x} S_{i+\hat{y},x} S_{i+\hat{y},y}. \quad (4.7)$$

From the model Eq.(4.5), we can immediately see the existence of the edge degree of freedom. As the Majorana fermions in bulk will be paired within the plaquette, there will be dangling Majorana fermions\footnote{113} at the boundary because of the edge cuts a plaquette in half (see Fig.4.1). It was already noticed\footnote{89 \footnote{113}} that this model (with $g > 0$) has a flat band of edge states on the boundary along $\hat{x}$- and $\hat{y}$- directional cut (see Fig.4.1). Hence, to look for gapless edge states for $Z_2$ spin liquids protected by translational symmetry, we can consider similar models which supports dangling Majorana fermions on the edge. We will generalize the structure of Wen’s model to generate a series of mean field Hamiltonian for $Z_2$ spin liquids with gapless boundary states in two and three spatial dimensions. We also discuss the stability of the gapless boundary states.
We now look into Wen’s model carefully. To illuminate the underlying structure of Wen’s model, we study the mean field Hamiltonian for the fermionic spinons (4.6).

\[ H_{\text{mean}}(\{f_{i,u}, f_{i,d}\}) = \sum_{ij} \left[ f_{i,\sigma}^{\dagger} u_{ij}^{\sigma,\tau} f_{i,\tau} + f_{i,\sigma} \eta_{ij}^{\sigma,\tau} f_{i,\tau} \right] + \text{h.c.} \]  

We notice, by plugging Eq.(4.6), that \( f_{i,u} \) and \( f_{i,d} \) are decoupled completely and form the one-dimensional Majorana fermion chains[115] (in the weak-pairing phase) along \( \hat{x} \)- and \( \hat{y} \)-axis. Explicitly, we now have

\[ H_{\text{mean}}(\{f_{i,u}, f_{i,d}\}) = h_{1D,\hat{x}}(\{f_{i,u}\}) + h_{1D,\hat{y}}(\{f_{i,d}\}), \]  

where \( h_{1D,\hat{n}}(\{f\}) \) is the one-dimensional Kitaev model along \( \hat{n} \) in the weak pairing regime. This explains why we have dangling Majorana fermions on the boundary along \( \hat{x} \)- and \( \hat{y} \)-directional cut of the lattice (See Fig.3.1). We will see that there is a gapless Majorana mode formed by the dangling Majorana fermions as long as there are odd number of Majorana fermions per unit cell on the edge. Before discussing the nature of the gapless edge states, we notice that we can easily generalize Wen’s model by deforming one of \( h_{1D,\hat{x}}(\{f\}) \) Eq.(4.9) into the trivial phase while keeping the constraint ‘one spinon per site’. Then, this Z2 spin liquid will break the \( C_4 \) rotational symmetry of square lattice while keeping the translational symmetry. For example, let us consider the case where \( h_{1D,\hat{x}}(\{f_{i,u}\}) \) is replaced by the trivial \( Q(\{f_{i,u}\}) \) (this Hamiltonian \( Q(\{f\}) \) is not necessarily one-dimensional but is fully gapped):

\[ H_{\text{mean}}(\{f_{i,u}, f_{i,d}\}) = Q(\{f_{i,u}\}) + h_{1D,\hat{y}}(\{f_{i,d}\}) \]  

has dangling Majorana fermions if the edge is not parallel to \( \hat{y} \). Similarly, we can generate a Z2 spin liquid which has dangling Majorana fermions if the edge is not parallel to \( \hat{x} \). For Z2A phase[32, 113] whose spinon band structure preserves translation symmetry explicitly, we can have another possible Z2 spin liquid where we align the Kitaev chain along \( \hat{n} = \hat{x} \pm \hat{y} \) (we will see later that this state has the same characteristics to the Wen’s model). Hence we have three translational symmetric Z2A spin liquids with the gapless edge states. Though these Z2A spin liquids have the same \( \mathbb{Z}_2 \) topological order and the same translational symmetry, we can distinguish them further by looking into the crystal momenta[89, 98] of the ground states and degeneracies, and the edge states. In the next section, we use these crystal momenta and degeneracies to find the effective BF theory for the Z2 spin liquids.

Now that we have some conditions for the existence of the edge states, we study their detailed features. We first discuss the relation between the edge degrees of freedom and the bulk gap. We argue that there is a gapless edge state as long as the bulk is gapped and the translational invariance at the edge remains unbroken (See Fig.4.2). To remove the boundary Majorana fermions, we need to pair them up into complex fermions. Due to the translational symmetry, a Majorana fermion on the boundary cannot pair up on the boundary if there is one single Majorana fermion per unit cell. What the Majorana fermion can do, instead of dimerizing on the boundary, is to tunnel through the bulk and
Figure 4.1: Illustration of Wen’s plaquette model and its edge state. (A) Plaquette operator $\prod_{<ij> \in P} U_{ij}$. A plaquette operator pairs up four Majorana fermions around the square. Here, blue circles represent four Majorana fermions per site, and red lines connecting two blue circles represent $U_{ij}$ appearing in the plaquette operator. (B) In terms of the complex fermions $f = \lambda \pm i\chi$ in Eq. (4.6), Wen’s plaquette model can be understood as the stacked one-dimensional Kitaev chains parallel to $\hat{x}$ and $\hat{y}$. (C) Edge states of Wen’s model where the edge is along $\hat{y}$ direction. The plaquette operators in Hamiltonian Eq. (4.5) cover all the Majorana fermions except a single Majorana fermion per site on the edge. The blue circles represent dangling Majorana fermions while red circles are Majorana fermions covered by the plaquette operators. These blue dangling modes will hop around by the magnitude $\sim t$ when we are away from the exactly solvable point. (D) The dangling Majorana fermions can be equally well understood via the stacked Kitaev chain picture. When the Kitaev chain is cut, the edge always hosts a single Majorana fermion per chain. It is clear that the edge states of (C) and (D) are exactly the same.
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pair-annihilate with the Majorana fermion on the opposite boundary. However, the tunneling length\cite{115} is $\sim 1/\sqrt{\Delta}$ where $\Delta$ is the bulk gap. Hence, we need to close the gap and go through the bulk phase transition to lose the dangling Majorana fermions at the boundary. In the next section, we will construct the effective $BF$ theory for these phases, and the effective theory should describe a finite range of the phase diagram as it is gapped and the edge state of the topological field theory is stable as long as the gap remains finite.

The above ‘gaplessness’ of the edge states depends on the number of Majorana fermions per unit cell on the boundary. If there are even numbers of the dangling Majorana fermions per unit cell, then Majorana fermions can pair up on the boundary without breaking the translational symmetry along the boundary. The ‘parity’ of the number of the dangling Majorana fermions on the arbitrary boundary can be easily computed, and there is an odd number\cite{116} of the dangling Majorana fermions per unit cell on the boundary if

$$J_{\hat{n}} = \frac{\hat{n}}{2} \cdot \vec{G} = \pi \mod 2\pi,$$

where $\hat{n}$ is the vector defined for the Hamiltonian of the Majorana fermion chain $h_{1D,\hat{n}}(\{f\})$, and $\vec{G}$ is the reciprocal vector orthogonal to the boundary. If there is more than one chain, we simply add up all $J_{\hat{n}} \mod 2\pi$. Then we have gapless edge modes protected by the translational symmetry if the sum is $\pi \mod 2\pi$. In fact, the same index is used to study the localized states at the dislocations of weak topological insulators/superconductors\cite{57,116}. Intuitively, $\hat{n} \cdot \vec{G}$ in Eq.(4.11) can be thought as the “flux density” of Kitaev chains (which are parallel to $\hat{n}$) passing through the area perpendicular to $\vec{G}$ (which is analogous to the definition of the flux through a surface in the elementary calculus, i.e., $F = \vec{E} \cdot \hat{S}$ defines the flux of the vector field $\vec{E}$ passing through the area perpendicular to the vector $\hat{S}$). Due to the ‘parity’ (or even/odd-ness) of the dangling Majorana fermions, we need to take mod by $2\pi$ with the appropriate normalization. To demonstrate this, we work out a few examples applying Eq.(4.11).

- example 1. edge state of Wen’s plaquette model with the edge parallel to $\hat{y}$. As the edge is along $\hat{y}$-direction, the reciprocal vector defining the edge is $\vec{G} = (2\pi, 0)$. In Wen’s plaquette model, we have the two Kitaev chains where each chain is identified with $\hat{n}_1 = (1, 0)$ and $\hat{n}_2 = (0, 1)$. We immediately have $J_{\hat{n}_1} = \pi$ and $J_{\hat{n}_2} = 0$ and thus we have a dangling Majorana fermion per site because $J_{\hat{n}_1} + J_{\hat{n}_2} \mod 2\pi = \pi$. This agrees with the previous intuitive understanding depicted in Fig.3.1.

- example 2. edge state of Wen’s plaquette model with the edge parallel to $\hat{x} + \hat{y}$. This edge can be identified with the reciprocal vector $\vec{G} = (2\pi, -2\pi)$. As before, we have the two Kitaev chains where each chain is identified with $\hat{n}_1 = (1, 0)$ and $\hat{n}_2 = (0, 1)$, and thus $J_{\hat{n}_1} = \pi$, $J_{\hat{n}_2} = -\pi$ and $J_{\hat{n}_1} + J_{\hat{n}_2} \mod 2\pi = 0$, i.e., there are even number of Majorana fermions per unit cell at the boundary and hence there is no gapless helical Majorana mode protected by the translational symmetry. Indeed, if we look at the edge defined by $\vec{G} = (2\pi, -2\pi)$, there are two Majorana fermions (per unit cell on the boundary) coming from the Kitaev chains along $\hat{x}$- direction and Kitaev chains along $\hat{y}$- direction on the boundary which immediately implies that there is no stable gapless edge state.
If we have a single Majorana fermion per unit cell, we can study the spectrum of the boundary modes. When the perturbation away from this ideal Hamiltonian is given, the dangling Majorana fermions will hybridize with the nearest neighbors and start to disperse

\[ H_{\text{edge}} = it \sum_j \eta_j \eta_{j+1}, \]

where the position of the boundary Majorana fermion is labeled by the index \( j \in \mathbb{Z} \) and \( t \) is the effective hopping parameters on the boundary. The spectrum of this Majorana fermion is given by \( E(k) = 2t \sin(k) \) for \( k \in (0, \pi) \) (this Majorana fermion problem is, in fact, related to the fermion doubling problem). To gap out the spectrum, we need a perturbation with a matrix element connecting \( k = 0 \) and \( k = \pi \). However, this interaction doubles the unit cell on the boundary (similar to the perturbations required to eliminate the surface of the weak topological insulator\[117, 118\]), and hence it is prohibited by the lattice translational symmetry. We note that the right-mover and the left-mover of the gapless edge theory have different center of mass momentum. This feature is also reproduced by the effective BF theory.

From this edge spectrum, the counting of Majorana fermions, and the translational symmetry, we now show that this edge theory mimics the stability of the edge state of a quantum spin Hall insulator against the coupling to ordinary one-dimensional Luttinger liquids. When the edge state of the spin Hall effect interacts with ordinary Luttinger liquids, the edge states are reconstructing themselves to the edge theory of spin Hall insulators with the renormalized coefficients. For the edge of the \( Z_2 \) spin liquids, we can couple our edge theory to the quantum Ising chain at the critical point, which is a gapless helical Majorana state (see Fig.4.2). The helical modes (the left-mover and the right-mover) of the quantum Ising chain are located at \( k = \pi \). When the helical modes are placed on top of the boundary Majorana modes of \( Z_2 \) spin liquids, the right-mover at \( k = 0 \) is intact as it cannot interact with the modes at \( k = \pi \). At \( k = \pi \), there are three modes (two from the critical Ising chain and one from the original QSH edge): one right-mover, two left-movers. The translational-invariant potential will have matrix elements connecting \( k = \pi \) to itself, allowing one right-mover and one left-mover to pair up. Hence, we are left with one left-mover at \( k = \pi \) which is reconstructed from the helical Majorana modes of the quantum Ising chain and the original left-mover at \( k = \pi \). Thus, the boundary remains gapless even if it interacts with the critical Ising chain. It is not difficult to see that other systems, such as helical Dirac edge, cannot gap out the original edge modes as they have even numbers of the helical Majorana fermions. The easiest way to understand this behavior is as follows; the size of the Hilbert space per site in the quantum Ising chain is 2, and we need two Majorana fermions per site to represent the Hilbert space. This implies that there are three Majorana fermions per unit cell (see Fig.4.2), and thus we expect the spectrum to be gapless after the dimerization of two of them. Hence we can conclude, based on the counting argument and the translational symmetry, that the edge is robust against to coupling to any one-dimensional gapless system.

It is also interesting to note that this edge spectrum implies that we will have a zero energy Majorana state at the lattice dislocation in \( Z_2 \) spin liquids\[116\]. For Wen’s plaquette
model, the dislocation of the Burger’s vector $\hat{x}$, $\hat{y}$ will trap the zero energy Majorana states. On the other hand, we will have the zero energy state of the Burger’s vector $\hat{m}$ orthogonal to $\hat{n}$ if Z2 spin liquids contains a Majorana fermion chain along $\hat{n}$ defined above in this section.

The discussion in this section is based on the mean field Hamiltonian for the Z2 spin liquids. However, the spectrum is fully gapped, and hence the fluctuation over mean field solutions are supposed to be small. Still, one might think that it is unclear if our result remains the same when both four-fermion interactions and gauge fluctuations are included. These questions, perhaps, cannot be answered in the mean field theory. Therefore we take a different path to answer the question. In the next section, we will find the effective $BF$ theory for these spin liquids, and the topological $BF$ theory should describe a phase instead of a point in the phase diagram. Hence the $BF$ theory predicts the phase to have gapless edge states on the boundary protected by translational symmetry as long as the gap remains finite.

### 4.3 Effective $BF$ theory and its characterization

In this section, we will construct the effective $BF$ theory of the Z2 spin liquids considered in the previous section. In previous studies [89, 113] it was shown that the translational symmetry restricts the form of the mass into the specific form so that the edge state becomes gapless. And the same effective theory captures the crystal momenta of the ground states and topological degeneracies in a square lattice with periodic boundary condition. Here we extend previous results in the way that we clarify the spectrum of the edge theory and its connection to the microscopic model discussed in the previous section (in fact, the spectrum of the edge states is crucial for the gaplessness as we saw in the microscopic discussion). Furthermore, we demonstrate the way of classifying $BF$ theory in the presence of lattice symmetries.

The essence of the effective theory is to encode the non-trivial transformations for the gauge fields in $BF$ theory (4.1) under translations (in the Coulomb gauge $a_0 = b_0 = 0$)

$$t_{x,y}: a_i \rightarrow b_i, \quad b_i \rightarrow a_i,$$

(4.13)

leaving the theory Eq.(4.1) invariant. $t_{x,y}$ denote lattice translations along $x$ and $y$ directions. This directly implies that the edge theory [89] should be symmetric under $\psi^\dagger_L \rightarrow \psi_L$ and $\psi_L \rightarrow \psi^\dagger_L$ in the edge theory Eq.(4.3). This symmetry, hence, restricts the form of the masses for the edge theory into

$$L_{\text{mass}} \sim a\psi^\dagger_R(\psi^\dagger_L + \psi_L) + h.c.,$$

(4.14)

To see the effect of this particular mass term Eq.(4.14), we introduce $\psi_R = \eta_R + i\chi_R$ and $\psi_L = \chi_L + i\eta_L$ where $\chi_R/L, \eta_R/L$ are real Majorana fermions. Then, the mass Eq.(4.14) gaps out $\chi_L$ and one of two right-moving Majorana modes $\chi_R, \eta_R$ (e.g. $\chi_R$ if $a$ is a real number), and hence we are left with one right-mover and one left-mover. It is not difficult to see $\eta_L$ is located at $k = \pi$ as $\psi_L$ transforms to $\psi^\dagger_L$ under unit lattice translation.
We will follow this lesson to construct and (partially) classify the effective $BF$ theory for the Z2 spin liquids discussed in the previous section. However, the classification in this section is based on the educated guesses constructed in the previous studies. The philosophy of this classification and characterization of $BF$ theory is, thus, phenomenological. Nevertheless, we will find the correct $BF$ theory for the Z2 spin liquids with the gapless edge states. More specifically, we will find that the $BF$ theory matches the crystal momenta and topological degeneracies, and the nature of the edge theories of Z2 spin liquids. This justifies the correctness of the effective $BF$ theories.

### 4.3.1 Crystal momenta and degeneracies of the Z2 spin liquids

To find $BF$ theory for the Z2 spin liquids, we first need to compute the crystal momenta and degeneracies for the spin liquids. We assume that the mean field Hamiltonian is enough for computing these quantities, i.e., the gauge fluctuation and interactions beyond the mean field states do not change the crystal momenta and degeneracies.

Here, we briefly show how to compute[89] the crystal momenta and degeneracies of the Z2 spin liquids. The calculation is based on the mean field theory for the Z2 spin liquids. In the mean field theory, we can assume that there are two fermions $\Psi^T = (\psi_1, \psi_2)$ per site. To connect to the spin-1/2 Hamiltonian, we identify $\psi_1 = f_\uparrow$ and $\psi_2 = f_\downarrow$ where $\uparrow/\downarrow$ denotes the spin up and down in basis of $S_z$, i.e., $\vec{S} = \frac{1}{2}\sum_{\alpha,\beta=\uparrow,\downarrow} f_{\alpha}^\dagger \sigma_{\alpha\beta} f_{\beta}$. This parton construction enlarges the Hilbert spaces $\{|\Psi_{\text{mean}}\rangle\}$, and we need to project it down to the physical states $\{|\Phi_{\text{spin}}\rangle\}$. The projection is given by

$$|\Phi_{\text{spin}}\rangle = P|\Psi_{\text{mean}}\rangle,$$

where $P$ projects the mean field state of fermions into the physical spin state with one fermion per site. In this paper, we specifically concentrate on the case of Z2 spin liquid, where the fluctuating gauge field is Z2 gauge field. According to projective symmetry group classification[32], there are two types of Z2 spin liquids if we have only translational symmetry: Z2A spin liquids (so-called zero flux states whose spinon band structure explicitly preserves translational symmetry) and Z2B spin liquids (so-called $\pi$-flux states whose spinon band structure doubles the unit cell). Here we focus on Z2A spin liquids. We introduce the fermion operator for $\Psi_k$ in the momentum space $\Psi_k = (\psi_{1,k}, \psi_{1,-k}, \psi_{2,k}, \psi_{2,-k})^T$ and write down the Hamiltonian for $\Psi_k$. Then, we see that $\Psi_k^\dagger \Psi_k = 2$ (number constraint) and $\Psi_k^\dagger \sigma^0 \otimes \sigma^3 \Psi_k = 0$ (particle-hole symmetry) for all $k$. In the presence of translational symmetry, phase transitions between different Z2 spin liquids happen when there is a level crossing at the high-symmetry points of the Brillouin zone[98]. There are four such points: $(0,0), (0,\pi), (\pi,0), (\pi,\pi)$. At these points, fermion occupation number $n_k \equiv \Psi_k^\dagger \sigma_3 \otimes \sigma_3 \Psi_k$ can take different values at these time-reversal-invariant momenta (TRIM) while $n_k = 2$ for all other possible $k$ in the Brillouin zone[89]. Different fillings at TRIM are the origin of the crystal momenta of Z2 spin liquids. The ground states can be obtained by filling all the
Figure 4.2: Stability of the gapless edge states. (A) To gap out the dangling Majorana fermions, the Majorana fermions should pair up and dimerize. However, it is clear from the figure that the dimerization doubles the unit cell along the boundary. This is similar to the physics of surface states of weak topological insulators\cite{117, 118}. (B) Coupling of the dangling Majorana fermions to the quantum Ising chain at criticality. As the Hilbert space per site of the Ising chain has the dimension $2 = (\sqrt{2})^2$, the Ising chain can be thought as the chains of two Majorana fermions per site. So when the Ising chain is coupled to the dangling Majorana fermions, there are three Majorana fermions per site which is guaranteed to be stable by counting Eq.\eqref{4.11}. (C) This picture can be further supported by looking at momentum space. The Ising chain at criticality is equivalent to a helical Majorana fermion state at $k = \pi$ and the edge state consist of the dangling Majorana fermions of the spin liquid has one mode at $k = 0$ and $k = \pi$. Thus there are total three modes at $k = \pi$ ($k = 0$ is decoupled from $k = \pi$ as the coupling between $k = 0$ and $k = \pi$ would double the unit cell). (D) When the interaction between the Ising chain and the edge state of the $\mathbb{Z}_2$ spin liquid is turned on, we will be left with one reconstructed Majorana mode at $k = \pi$ and another mode at $k = 0$. 
states below the chemical potential $\mu = 0$ (half-filled). Hence the ground state carries the crystal momentum depending on the filling $n_k$ at these high-symmetry points.

Naively, there are four ground states for a $\mathbb{Z}_2$ spin liquid on the torus, and the four ground states can be labelled by the boundary conditions along the two directions of the torus (the four ground states are generated by imposing ‘periodic’ $\times$ ‘periodic’, ‘periodic’ $\times$ ‘anti-periodic’, ‘anti-periodic’ $\times$ ‘periodic’, ‘anti-periodic’ $\times$ ‘anti-periodic’ boundary conditions along the two directions of the torus to the fermions). As the total number of the fermions in the periodic', 'anti-periodic', $i.e.,$ TRIM $n$ because $n_{k} = 2$ for all $k \in BZ \setminus \text{TRIM}$ [89]. However, not all of $k \in \text{TRIM}$ is allowed for the fermion. For example, on the odd-by-even lattice (with the size of the system $N_x \times N_y$ such that $N_x \in 2\mathbb{Z} + 1$ and $N_y \in 2\mathbb{Z}$) with the periodic boundary conditions along the two directions of the torus, the allowed momenta $(k_x, k_y)$ for the fermions can take the values of $(\frac{2\pi n_x}{N_x}, \frac{2\pi n_y}{N_y})$ with $n_x = 0, 1, 2, \cdots N_x - 1, N_x$ and $n_y = 0, 1, 2, \cdots N_y - 1, N_y$. In this case, there is no allowed state for the fermions at $k = (\pi, 0)$ and $(\pi, \pi)$, and thus the summation $\sum_{k \in \text{TRIM}} n_k$ should be modified to the summation $\sum_{k \in \text{TRIM}^*} n_k$ where $\text{TRIM}^*$ is the set of the allowed momenta among $k \in \text{TRIM}$. On the other hand, if the boundary condition along $\hat{x}$-direction is changed to be anti-periodic while keeping the boundary condition along $\hat{y}$ - direction periodic, then the allowed momenta $(k_x, k_y)$ is changed to $k_x = \frac{2\pi}{N_x}(n_x + \frac{1}{2}), n_x = 0, 1, 2, \cdots N_x$ with $k_y$ as before. For this case, $\text{TRIM}^*$ is identical to $\text{TRIM}^*$ i.e., $\text{TRIM}^* = \{(0, 0), (\pi, 0), (0, \pi), (\pi, \pi)\}$.

In the given lattice with the specified boundary condition, we can compute the sum $\sum_{k \in \text{TRIM}^*} n_k$ for a $\mathbb{Z}_2$ spin liquid. If $\sum_{k \in \text{TRIM}^*} n_k \in 2\mathbb{Z} + 1$, then the state labelled by the boundary condition is not a physical state and the state should not be considered as one of the ground states. Thus, the number of the ground states on the lattice can be smaller than the naive expectation 4 on torus. When $\sum_{k \in \text{TRIM}^*} n_k \in 2\mathbb{Z}$, then the crystal momenta for the state is given by $\sum_{k \in \text{TRIM}^*} k n_k$. Hence, if a $\mathbb{Z}_2$ spin liquid is given, we can compute the number of ground states on the four lattices (even-by-even, even-by-odd, odd-by-even, and odd-by-odd lattices) and label the ground states of the four lattice with the crystal momenta. For example, there are only two ground states for Wen’s plaquette model on the even-by-even lattices, and the two states carry the crystal momenta $(0, 0)$ obtained by computing $\sum_{k \in \text{TRIM}^*} k n_k$ for the two ground states. We can write this compactly as follows (we denote “e×o” lattice as even-by-odd lattice)

(ex) Wen’s plaquette model

$e \times o$ lattice: $(0, 0), (0, 0)$

Following the above discussion, we find the crystal momenta of the ground states for the three $\mathbb{Z}_2$ spin liquids in the previous section (here we again denote “e×e lattice” as even-by-even lattice, and “e×o lattice” as even-by-odd lattices, etc.)
(1) Wen’s plaquette model, and \( \hat{n} = \hat{x} \pm \hat{y} \)
  - exe lattice: \((\pi, \pi), (0, 0), (0, 0), (0, 0)\)
  - exo lattice: \((0, 0), (0, 0)\)
  - oxe lattice: \((0, 0), (0, 0)\)
  - oxo lattice: \((0, 0), (0, 0)\)

(2) \( \hat{n} = \hat{x} \)
  - exe lattice: \((0, \pi), (0, 0), (0, 0), (0, 0)\)
  - exo lattice: \((0, 0), (0, 0)\)
  - oxe lattice: \((0, \pi), (0, 0), (0, 0), (0, 0)\)
  - oxo lattice: \((0, 0), (0, 0)\)

(3) \( \hat{n} = \hat{y} \)
  - exe lattice: \((\pi, 0), (0, 0), (0, 0), (0, 0)\)
  - exo lattice: \((\pi, 0), (0, 0), (0, 0), (0, 0)\)
  - oxe lattice: \((0, 0), (0, 0)\)
  - o xo lattice: \((0, 0), (0, 0)\)

We will see that this complicated pattern of the crystal momentum can be reproduced by the effective BF theory in the next subsection. While deriving the above result, we implicitly assumed that the Hamiltonian \( Q(\{f\}) = \pm 1 \) for the trivial chain not to have any potential structure in it. While the Hamiltonian \( Q \) here is artificial, we need to close the gap at the high-symmetry points of the Brillouin zone to change the crystal momenta. Hence, the pattern of the crystal momenta should be properties of a phase, not of a point in the phase diagram.

### 4.3.2 Classification of BF theory on the square lattice with translational symmetry

To classify BF theory, we begin with the lesson from the previous studies\[^{89, 113}\] that we will utilize in this section. The first lesson is that encoding the transformation on the gauge theory is not 'gauge' degree of freedom, but it is a physical symmetry. For example in the toric code or Wen’s plaquette model, we exchange the electric excitation and the magnetic excitation under the translation. This is different from \( SL(2; \mathbb{Z}) \) gauge symmetry for BF theory. The second lesson is that we can obtain the complicated patterns for the crystal momenta and degeneracies by implementing the non-trivial transformations. Hence, the strategy is simple: finding all the possible physical transformations for BF field theory. In the following discussion, we will systematically search and implement the transformations for BF theory.

We begin with the Coulomb gauge \( a_0 = b_0 = 0 \) for the gauge fields \( a_\mu \) and \( b_\mu \) in Eq.(4.1).
Then, this reduces Eq. (4.1) into the following form (without sources)

\[ L = \frac{1}{2\pi} v^T \cdot J \cdot \partial_0 v \]  

(4.16)

where \( v^T = (a_x, a_y, b_x, b_y) \) and

\[ J = \begin{bmatrix} 0 & 0 & 0 & +1 \\ 0 & 0 & -1 & 0 \\ 0 & +1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix} \]  

(4.17)

To be invariant under a unit lattice translation \( t_x \) in \( x \)-axis (and similar for \( t_y \) in \( y \)-axis), we require

\[ L = \frac{1}{2\pi} v^T \cdot J \cdot \partial_0 v = \frac{1}{2\pi} (t_x [v^T]) \cdot J \cdot \partial_0 (t_x [v^T]). \]  

(4.18)

Hence, we look for solutions \( t_x \) and \( t_y \) satisfying Eq. (4.18). The obvious possibility for \( t_x \) and \( t_y \) is to consider the linear transformations acting on \( v \), i.e., we associate \( (t_x, t_y) \) with the matrices \( (O_x, O_y) \) and the vectors \( (u_x, u_y) \) such as

\[ t_{x,y} : v \rightarrow O_{x,y} v + u_{x,y}. \]  

(4.19)

We plug this into Eq. (4.18) and find a restriction on \( O_{x,y} \)

\[ O_{x,y}^T J O_{x,y} = J, \]  

(4.20)

The restriction for \( u_{x,y} \) shows up when we take the microscopic picture into consideration.

Before proceeding further, we notice that \( O_{x,y} \) is orthogonal, i.e., \( \det(O_{x,y}) = \det(O_{x,y}^T) = \pm 1 \) as \( J \) is invertible. This alone cannot fix the form of \( O_{x,y} \). We also note that \( O_{x,y}^2 = 1 \). This is because the size of the smallest even-by-even lattice is \( 2 \times 2 \), and we expect the degeneracies on the even-by-even lattice are trivially 4 i.e., we force the gauge field \( v \) to return to itself.

Then, it is easy to check that there are four solutions for \( O_{x,y} \) satisfying Eq. (7.20) (Note that the overall sign of the \( O_{x,y} \) is irrelevant as the sign of \( Z_2 \) theory is not important). The first physical solution is the trivial \( I = \text{diag}(1, 1, 1, 1) \). The second physical solution is ‘twist’ \( O^t \)

\[ O^t = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \]  

(4.21)

which exchanges \( a_i \) and \( b_i \), i.e., \( a_i \rightarrow b_i \) and \( b_j \rightarrow a_j \) under a unit lattice translation. The third possible (but not physical) solution \( Q \) is

\[ Q = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \]  

(4.22)
which acts as \((a_x, b_x) \to (a_y, -b_y)\) and \((a_y, b_y) \to (a_x, -b_x)\). The fourth non-physical solution \(P\) is

\[
P = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1 \\
\end{bmatrix}
\] (4.23)

which flips the sign of \(a_y\) and \(b_x\) spontaneously. A physical argument for excluding \(P\) and \(Q\) comes from the coupling of \(BF\) fields to the \(\mathbb{Z}_2\) charge field \(z\) and the \(\mathbb{Z}_2\) vortex field \(v\). We have the full Lagrangian \(L = L_{BF} + L_{\text{coup}}\) where \(L_{BF}\) is Eq. (4.16) and (in the Coulomb gauge \(a_0 = b_0 = 0\))

\[
L_{\text{coup}} = |(\partial_j - ia_j)z|^2 + |(\partial_j - ib_j)v|^2,
\] (4.24)

Now, we translate the system by one unit lattice along \(x\)-axis which acts as \(t_x\) on the fields. Here, \(t_x [\partial_j] = \partial_j\) and \(t_x [L_{BF}] = L_{BF}\), and we are required to satisfy the equation \(L_{\text{coup}} = t_x [L_{\text{coup}}]\) where

\[
t_x [L_{\text{coup}}] = |(\partial_j - it_x [a_j])t_x [z]|^2 + |(\partial_j - it_x [b_j])t_x [v]|^2.
\] (4.25)

For \(t_x = I\), we have \(t_x : z \to z\) and \(t_x : v \to v\). For \(t_x = O^1\), we have \(t_x : z \to v\) and \(t_x : v \to z\). However, for \(P\) and \(Q\), there is no way to make the equality \(t_x [L_{\text{coup}}] = L_{\text{coup}}\) from \(t_x [z]\) and \(t_x [v]\), hence we exclude them as the physical transformation of \(BF\) theory which is consistent with the \(\mathbb{Z}_2\) spin liquids in the previous section.

Now, we move on to the constant vector \(u_{x,y}\). As the vectors \(v\) are \(\mathbb{Z}_2\) gauge theory in the microscopic picture, so should be \(u_{x,y}\). More specifically, \([u_{x,y}]_{u} \in \{0, \pi\} \mod 2\pi\). However, not all of \(u_{x,y}\) pattern are physically independent. There are \(\pi\) flux or no flux in \(\mathbb{Z}_2\) gauge theory for \(a_i\) and \(b_j\), and this reduces many \(u_{x,y}\) patterns into only four of them. Those are the followings: 1) Both \(a_{\mu}\) and \(b_{\nu}\) have fluxes in the unit cell. 2) only \(a_{\mu}\) contains fluxes in the unit cell. 3) only \(b_{\nu}\) contains fluxes in the unit cell. 4) No fluxes are present. For 1), we have \(u^T_x = (0, \pi, 0, 0)\) and \(u^T_y = (0, 0, \pi, 0)\). For 2), we have \(u^T_x = (0, \pi, 0, 0)\) and \(u^T_y = (0, 0, 0, 0)\). For 3), we have \(u^T_x = (0, 0, \pi, 0)\) and \(u^T_y = (0, 0, 0, 0)\). For 4), we have \(u^T_x = u^T_y = (0, 0, 0, 0)\).

We write \((t_x, t_y)\) as \(\{(O_x, u_x), (O_y, u_y)\}\). We denote twist matrix simply as \(O^i\) and trivial matrix as \(I\), and we also denote the nontrivial flux vector as \(u\) and no flux as \(0\). For example, we can have \(BF\) theory with the translational invariant property \(\{(O^i, 0), (I, u_y)\}\) satisfies the following relations: \(t_x : (a_i, b_j) \to (b_i, a_j)\) and \(t_y : (a_i, b_j) \to (a_i, b_j + \pi \delta_{xj})\).

A simple combinatorial computation then concludes that this classification gives \(2 \times 2 \times 4 = 16\) classes for \(BF\) theory consistent with the underlying \(\mathbb{Z}_2\) gauge theory on the square. Among 16 classes, six classes are not of interest. To see this, we look at the commutation relation for \(t_x\) and \(t_y\)

\[
[t_x, t_y] \neq 0
\] (4.26)

seemingly implying that those states are not physical. But this is not true; for example, the magnetic translations are not commuting each other in the quantum Hall states. Still, there is no allowed ground state in the odd-by-odd lattices if \([t_x, t_y] \neq 0\). As all of our targeting states have 2 or 4 states, we exclude the \(BF\) theory of \([t_x, t_y] \neq 0\).
4.3.3 Crystal momenta, degeneracies, and Z2 indices

Upon obtaining the transformations for the relevant BF theory, we compute the crystal momenta of the ground states on even-by-even, odd-by-even, even-by-odd, and odd-by-odd lattices. We follow the straightforward calculation in the reference [59] to get the crystal momenta.

Before presenting a series of results from the computation, we exhibit two examples showing how we get the crystal momenta on lattices.

Example 1. \{\langle \mathbf{I}, \mathbf{u} \rangle, \langle \mathbf{I}, \mathbf{0} \rangle\}
We have the transformations under the translations as \(t_x : (a_i, b_j) \to (a_i + \pi \delta_{y,i}, b_j)\) and \(t_y : (a_i, b_j) \to (a_i, b_j)\). We denote the zero mode of BF fields \((a_i, b_j)\) as \(\langle \theta_i, \phi_j \rangle\). Then, the BF theory relates \(\theta_x (\phi_x)\) to \(\phi_y (\theta_y)\) as the canonical conjugate pairs. Explicitly, we have \([\theta_x, \phi_y] = i\pi\) and \([\phi_x, \theta_y] = i\pi\). Then, we have four well-defined ground states \(\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\}\) such as \(\{2\rangle = e^{-i\theta_x}\{1\rangle, \{3\rangle = e^{-i\phi_x}\{1\rangle, \{4\rangle = e^{-i\theta_x}e^{-i\phi_x}\{1\rangle\) where \(\{1\rangle\) transforms trivially under any transformations of \(t_{x,y}\). Then, we have \(t_x : (\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\) \to (\{3\rangle, \{4\rangle, \{1\rangle, \{2\rangle\) and \(t_y : (\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\) \to (\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\). Hence, \([t_x, t_y] = 0\) and \(t_x\) and \(t_y\) can be simultaneously diagonalized. We conclude that the two states of the form \(\frac{1}{\sqrt{2}}(\{1\rangle - \{3\rangle\) and \(\frac{1}{\sqrt{2}}(\{2\rangle - \{4\rangle\) carry the crystal momentum \((\pi, 0)\), and other two states carry the crystal momentum \((0, 0)\) for any lattice. This gives the crystal momentum spectrums \((\pi, 0), (\pi, 0), (0, 0), (0, 0)\) on even-by-even, even-by-odd, odd-by-even, and odd-by-odd lattices, and there is no matched Z2 spin liquids of interest.

Example 2. \{\langle \mathbf{O}^t, \mathbf{0} \rangle, \langle \mathbf{I}, \mathbf{0} \rangle\}
We have the transformation law under the translations \(t_x : (a_i, b_j) \to (b_i, a_j)\) and \(t_y : (a_i, b_j) \to (a_i, b_j)\). We begin with the even-by even lattice. Then, we can expand BF theory and obtain the zero modes \(\theta_x (\phi_x)\), canonical conjugate to \(\phi_y (\theta_y)\). Then as before, we have four well-defined ground states \(\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\}\) such as \(\{2\rangle = e^{-i\theta_x}\{1\rangle, \{3\rangle = e^{-i\phi_x}\{1\rangle, \{4\rangle = e^{-i\theta_x}e^{-i\phi_x}\{1\rangle\) where \(\{1\rangle\) transforms trivially under any transformations of \(t_{x,y}\). Then, we have \(t_x : (\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\) \to (\{1\rangle, \{3\rangle, \{2\rangle, \{4\rangle\) and \(t_y : (\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\) \to (\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\). Hence, \([t_x, t_y] = 0\) and \(t_x\) and \(t_y\) can be simultaneously diagonalized. We conclude that one state of the form \(\frac{1}{\sqrt{2}}(\{2\rangle - \{3\rangle\) carries the crystal momentum \((\pi, 0)\), and the other three states carry the crystal momentum \((0, 0)\) for even-by-even lattice. This gives the spectrum of the crystal momenta \((\pi, 0), (0, 0), (0, 0), (0, 0)\) on even-by-even lattice. Now, we move to the even-by-odd lattice. In this case, we can expand the zero mode as well as in even-by-even lattice because \(t_y\) is trivial, and this gives the crystal momentum spectrum \((\pi, 0), (0, 0), (0, 0), (0, 0)\) on even-by-odd lattice. It turns out to be different for odd-by-even lattice as the non-trivial boundary condition \(T_x : (a_i, b_j) \to (b_i, a_j)\) where \(T_x = (t_x)^{T_x}\), and we cannot expand BF theory to obtain the zero mode. The resolution for this is to double the odd-by-even lattice along \(x\) axis to get even-by-even lattice. Then, we can now expand BF fields to obtain the zero modes \(\{1\rangle, \{2\rangle, \{3\rangle, \{4\rangle\}\) such as \(\{2\rangle = e^{-i\theta_x}\{1\rangle, \{3\rangle = e^{-i\phi_x}\{1\rangle, \{4\rangle = e^{-i\theta_x}e^{-i\phi_x}\{1\rangle\) with the boundary condition \(T_x : (\theta_x, \phi_x) \to (\phi_x, \theta_x)\). The boundary condition implies that the
originally four independent states bind to each other to form only two independent states $|1\rangle, |2\rangle$. Furthermore, $t_x : (|1\rangle, |2\rangle) \rightarrow (|1\rangle, |2\rangle)$, and thus the crystal momentum spectrum on the odd-by-even lattice is $(0, 0), (0, 0)$. The similar consideration on odd-by-odd lattice gives the crystal momentum spectrum as $(0, 0), (0, 0)$. These crystal momentum spectrums match the spin liquids of $\hat{n} = \hat{y}$ in the previous section.

This calculation can be also done for other translational symmetric $BF$ theory, and now we find that

1. $\{(O, 0), (O, 0)\}$ is Wen’s model or $\hat{n} = \hat{x} \pm \hat{y}$
2. $\{(O, 0), (I, 0)\}$ is $\hat{n} = \hat{y}$ Z2 spin liquid
3. $\{(I, 0), (O, 0)\}$ is $\hat{n} = \hat{x}$ Z2 spin liquid

It is not difficult to see that these $BF$ theories have the same edge spectrum as the microscopic consideration in the previous section. The spectrum of the crystal momenta and degeneracies for other $BF$ theories can be found in the appendix [10].

Before finishing this section, we comment on the connection to the previous study [98]. The pattern of the crystal momenta and degeneracies of Z2 spin liquids are, in fact, fixed by the fermion parity at the high symmetry points in the Brillouin zone, and this fact can be used to classify Z2 spin liquids. We can find that Wen’s model and $\hat{n} = \hat{x} \pm \hat{y}$ belong to [0110] and [1001] classes in the classification of Z2 spin liquids in the index system of the previous study ($\hat{n} = \hat{x}$ belongs to [1100] and [0011] classes, and $\hat{n} = \hat{y}$ belongs to [1010] and [0101] classes.) Though it can be shown that these Z2 spin liquids with the gapless edge belong to the particular class, it is not clear if this index system implies the gapless edge states between Z2 spin liquids and vacuum. It would be an interesting future direction to study if the indices imply the presence of the gapless edge state.

### 4.4 Generalizations and Conclusions

Can we generalize our reasoning for the gapless edge states of Z2 spin liquids on the square lattice to other lattices such as the triangular lattices? More interestingly, can we generalize it to higher dimensions? It is not difficult to note that the answers to these questions are ‘yes’, at least in the mean field Hamiltonian. The nature of the edge states will depend on the direction of stacking one-dimensional Majorana fermion chains for $f_{i,u}$ and $f_{i,d}$. Hence, we can apply this to any two-dimensional lattice to construct Z2 spin liquids with the gapless edge states. We can also generalize to three-dimensional spin liquids to write down the mean field Hamiltonian, but it is better to have an exactly solvable model that exhibits the gapless surface states for the cubic lattice. The model is the direct generalization of Wen’s plaquette model on the square lattice, and it involves six Majorana fermions per site, i.e., this is a Hamiltonian for a spin-3/2 system [119]. We start with the Z2 gauge theory on the cubic
where $P$ denotes the plaquette of the cubic lattice. Here, $U_{ij} = \pm 1$ is the $\mathbb{Z}_2$ gauge on the link $<ij>$, and thus $\prod_{<ij> \in P} U_{ij} = F_P$ is the field strength on the plaquette $P$. The particular (but general) representation of this gauge theory is $U_{i,i}^{\hat{x}} = i\lambda_{i,x} \chi_{i}^{\hat{x}}$, $U_{i,i}^{\hat{y}} = i\lambda_{i,y} \chi_{i}^{\hat{y}}$, $U_{i,i}^{\hat{z}} = i\lambda_{i,z} \chi_{i}^{\hat{z}}$ with the translational symmetry. Hence, we have the six Majorana fermions $(\lambda_{i,x}, \lambda_{i,y}, \lambda_{i,z}, \chi_{i,x}, \chi_{i,y}, \chi_{i,z})$ per site, and the dimension of the Hilbert space per site is $2^6/2 = 8$ states per site. Again we need to halve this Hilbert space to represent a spin-3/2 system, i.e., the Hilbert space per site should be 4. This is done by taking the $\mathbb{Z}_2$ redundancy into account: Eq. (4.27) is invariant under $U_{ij} \rightarrow s_i U_{ij} s_j$, $s_i = \pm 1$.

In the three-dimensional model, we see that all the Majorana fermions in the bulk are paired. On the boundary, however we have one dangling Majorana fermion per unit cell on the boundary. Following the reasoning in the two-dimensional system, the flat bands on the boundary will start to disperse to form the gapless surface states when a small perturbation away from this exactly solvable limit induces

$$H_{edge} = i \sum_i (t_x \eta_i \eta_i^{\hat{x}} + t_y \eta_i \eta_i^{\hat{y}}).$$

This Hamiltonian has the gapless spectrum $E(k) = \sqrt{t_x^2 \sin^2 (k_x) + t_y^2 \sin^2 (k_y)}$. To gap out the spectrum, we need to double the unit cell[117, 118] which is prohibited by the translational symmetry.

As before, we can deform the exactly solvable Hamiltonian to obtain a series of anisotropic $\mathbb{Z}_2$ spin liquids with the gapless surface states. How many different classes of the $\mathbb{Z}_2A$ spin liquids with translational symmetry in the cubic lattice are there (if two $\mathbb{Z}_2$ spin liquids have the same crystal momentums and degeneracies, and the surface states, we define them as the same class)? We repeat the argument in the two-dimensional case and construct 3D mean field (ideal) Hamiltonians of $\mathbb{Z}_2$ spin liquids from the one-dimensional Majorana fermion chains. By checking the crystal momenta and the degeneracies in the three-dimensional lattices, we found that there are 14 classes which have the gapless surface states protected by the translational symmetry. The effective theory for these $\mathbb{Z}_2$ spin liquids should be (3+1)-dimensional $BF$ theory[52]

$$L = \frac{1}{2\pi} b_{\mu\nu} \partial_\lambda a_\rho - \frac{1}{2} \Sigma^{\mu\nu} b_{\mu\nu} - a_\mu j^\mu,$$

which is known to have the gapless Dirac-like surface spectrum[39]. It would be an interesting future research direction to show how the translational invariance stabilizes the gapless surface states of (3+1)-dimensional $BF$ theory.

In summary, we considered translationally-symmetric $\mathbb{Z}_2$ spin liquids which have gapless edge/surface states. The edge/surface states are constructed out of the dangling Majorana fermions on the boundary. We clarified the conditions for the gapless edge states for $\mathbb{Z}_2$
spin liquids and constructed the effective $BF$ theory reflecting the underlying translational symmetry of the lattice. The general reasoning applies to the three-dimensional lattices, and we demonstrated that there is a gapless surface state.

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Chapter 5

Quantum phase transition and fractional excitations in a topological insulator thin film with Zeeman and excitonic masses

The surface states of three-dimensional topological insulators (TI) are two-dimensional metals with an odd number of Dirac points enclosed by the Fermi surface\(^6\)\(^8\)\(^83\). They avoid the so-called fermionic doubling problem and are known in several cases\(^21\)\(^120\)\(^121\) to support topological correlated states when different types of interactions are added. The example motivating this paper is the topological exciton condensate formed by the Coulomb interaction between top and bottom surfaces of a thin film of topological insulator\(^121\). The exciton condensate on the TI surfaces carries electronic charge \(\pm \frac{1}{2}e\) at its vortices, i.e., half of the charge of the underlying electrons. This thin TI exciton condensate should be compared to that in a graphene bilayer, which has similar relativistic electronic structure to a TI surface. The fractional properties are washed out by the spin/pseudospin degeneracies in graphene. For example, the Kekulé vortex on graphene can support fractional quantum numbers\(^122\)\(^124\), but the fractional excitation should be multiplied by 4 (or 2, depending on how the degeneracies are lifted) and results in integral quantum numbers as for electrons. (See also the charge fractionalization on the kagome lattice\(^125\) at filling 1/3)

In the thin film, we have at least two Dirac fermions overall, one from the top surface and one from the bottom, and hence the system looks “ordinary” in the sense that we have an even number of fermionic degrees of freedom. However, it still has only half as many degrees of freedom as graphene, and it is known from previous work that the Topological Exciton Condensate (TEC) is distinct from an ordinary BEC of excitons. It is fractional in the sense that it supports charge \(\pm \frac{1}{2}e\) at its vortices\(^121\). This fractional quantum number of TEC results from the topological structure of the TI. Now the TEC is \(T\)-symmetric but generates a mass at the Dirac points. One way to motivate the present work is to compare this effect to the easiest way to open up a gap at the Dirac points of TI surface, namely, to break
Section 5.1. Microscopic model and band structure

$T$-symmetry on the surface. There are a few natural ways to break $T$-symmetry and open up gaps at Dirac points: coating magnetic materials, or imposing magnetic fields etc. Thus if we introduce $T$-symmetry breaking perturbation and condense $T$-symmetric excitons on TI surfaces at the same time, then we expect that there should be an interesting interplay between TEC mass and $T$-symmetry breaking masses. We find a quantum phase transition (QPT) between two phases that can be labeled by the behavior of their quasiparticles: Quantum Anomalous Hall (QAH) and Quantum Spin Hall (QSH) phases.

Here, we will first consider a thin TI film coated by ferromagnets (FM) on both sides (Fig. 5.1). Then the system is gapped due to the $T$-breaking perturbation of the originally gapless surface. The electrons on the TI surface interact with the FM magnetization via Zeeman coupling $J_H \sigma \cdot M$. The $z$-component magnetization has a special role: it opens up a gap at the Dirac point with mass $J_H |M_z| \text{sgn}(M_z)$. This coupling is different from the case of graphene, where the pseudospins do not interact with magnetization and the Zeeman effect does not open up a gap. Other components of $M$ act as external gauge fields coupled to the Dirac fermions. When the system is fully gapped, we can safely integrate out fermions and obtain effective field theories for the gauge fields. We will develop the field theories for the fluctuating gauges and vortices in the two distinct phases. Even though the physics is most transparent when only the Zeeman coupling is considered, the same physics applies even when we consider an external $z$-directional magnetic field. The key difference in this case is that we have Landau levels (LL) instead of a Dirac spectrum. Despite this, we still have fractional vortices and a quantum phase transition when the Zeeman energy is comparable to TEC mass.

The following section studies the electronic band structure and shows that there is a QPT when the Zeeman mass is comparable to the exciton mass. At the QPT, the gap vanishes and the topological invariant (Chern number) of the bands is changed, which is why we refer to the transition as between QSH and QAH phases. In Section III we obtain an effective field theory that captures the topological properties. From this we can derive information about the change across the transition in the charge, statistics and the number of bound zero modes in a vortex. We next proceed to the uniform magnetic field case and find generally similar physics as in the Zeeman case. We also present the solution of the fermion zero mode at the vortices. In QSH, there is only one fermionic zero mode which disappears at the quantum phase transition to QAH. However, it is difficult to obtain the exact solution for the fermionic zero mode in the uniform orbital magnetic field but we show that we can manage to obtain analytic solutions for some limiting cases. In closing we discuss experimental detection of the phase transition and conditions required to observe the exciton condensate.

5.1 Microscopic model and band structure

We start from a microscopic model of a thin TI with a $T$-breaking Zeeman mass induced by proximity to a ferromagnet. We have two Dirac cones indexed by $\alpha = 1, 2$ (layer index) and short-ranged Coulomb interactions $U, V$. Here we specialize to the case $M_x \sim M_y \ll M_z$. 
Figure 5.1: A. Illustration of a thin topological insulator film sandwiched between ferromagnetic layers. To see the quantum phase transition between quantum spin Hall (QSH) and quantum anomalous Hall (QAH) phases, we need to align the magnetism along the same direction on both layers. B. Alternate experimental scheme. We sandwich a thin ferromagnetic layer between two bulk topological insulators. If we put an insulator with small dielectric constant $\epsilon$ instead of ferromagnets, we expect to observe an increased critical temperature for the superfluid - insulator transition into the excitonic condensate.

We include external EM probe fields $A_i$ which couple to the Dirac fermions and ignore the tunneling between layers, as this decays exponentially in thickness whereas the Coulomb energy decays only algebraically. For simplicity we set the chemical potential $\mu = 0$ (however, the topological properties studied here should be valid whenever the chemical potential is in the gap) and start from the weak Coulomb interaction where no phase transition is expected:

$$H = \sum_{\alpha=1,2} ((-1)^\alpha v_F \sigma \cdot (p - eA) + J_H M^2 \sigma^z + U n_\alpha n_\alpha) + V n_1 n_2$$  \hspace{1cm} (5.1)
Here $\sigma$ are the Pauli matrices for (physical) spin. Ignoring $U = \frac{e^2}{d^3}$ (where $l$ is the system-dependent length of short-ranged Coulomb interaction) and $V = \frac{e^2}{d^3}$ (where $d$ is the width of the thin film), we can easily identify the eigenstates and eigenvalues of $H$. This is reasonable as $U$ and $V$ will only renormalize the Dirac velocity when they are small. From here onwards, we rescale $v_F = 1$ as this should not change topological properties. With this in mind, we rewrite the Hamiltonian in a more familiar format $H = F^\dagger HF$ where $F$ is the four-spinor for the system:

$$H = \begin{bmatrix}
  m & p_+ & 0 & 0 \\
  p_- & -m & 0 & 0 \\
  0 & 0 & m & -p_+ \\
  0 & 0 & -p_- & -m
\end{bmatrix}$$

(5.2)

There are two important points to note about this Hamiltonian $H$. First, the Hamiltonian has the spectrum with the gap $2|J_H M_z = m|$ at the Dirac point.

$$E_{p,s} = \text{sgn}(s)\sqrt{p^2 + m^2}, \quad s = \pm 1$$

(5.3)

The spectrum is doubly degenerate due to the layer index. Moreover, from the matrix form (5.2) of $H$, we identify both up and down layers as in a QAH phase. To see this, let us take only the upper half of the block Hamiltonian $H_u$ such that

$$H = \begin{bmatrix}
  H_u & 0 \\
  0 & H_d
\end{bmatrix}, \quad H_u = \begin{bmatrix}
  m & p_+ \\
  p_- & -m
\end{bmatrix} = p \cdot \sigma + m \sigma_z$$

(5.4)

Now, we compute the winding number for $H_u = p \cdot \sigma + m \sigma_z$. We identify the vector $V_u = (p_x, p_y, m)$ from $H_u$, and compute the topologically invariant winding number (the first Chern Number) for $V$ by evaluating

$$C_1 = \frac{1}{4\pi} \int dp_x \int dp_y \hat{V} \cdot \frac{\partial \hat{V}}{\partial p_x} \times \frac{\partial \hat{V}}{\partial p_y}$$

(5.5)

where $\hat{V} = V/|V|$. The winding numbers for $H_u$ and $H_d$ are $\text{sgn}(m)\frac{1}{2}$ which reflects the origin of the anomalous quantum Hall effect for the Dirac fermions. Taken as a whole, the system is in a QAH regime where the Hall conductance is quantized as $\frac{e^2}{h}$.

So far, we have neglected the Coulomb interactions as they only renormalize parameters when they are small. However, when the Coulomb interaction increases, there can be phase transitions to a stripe phase [126] for strong $U$, or exciton condensate [121] for strong $V$. We are interested here in the TEC which is $T$-symmetric but still opens up a gap. To obtain TEC, we treat $V$ in terms of Mean Field Theory (MFT) in the exciton order parameter and ignore $U$. We do the MFT for $V_{n_1n_2} = f_{\sigma}^1 M^{\sigma\rho} f_{\rho}^2 + h.c$ with $M^{\sigma\rho} = <f_{\sigma}^1 f_{\rho}^{2\dagger}>$ (where $f_{\sigma}^1$ and $f_{\rho}^2$ are two-component Dirac fermions for layer 1 of spin $z$-component $\sigma$ and 2 of spin $z$-component $\rho$). Here, different $M$ describes different exciton condensates but we will choose an $M$ which opens up a gap at the Dirac points and is $T$-symmetric [121]. The order is described by $M = \Delta \tau^z \sigma^0$ where $\tau$ are Pauli matrices acting on layer index, and $\sigma$ acts on
spin as before. With the exciton order parameter, we have the following second-quantized mean field Hamiltonian.

\[ H = \sum_{\alpha} f_{\alpha}^\dagger (\sigma^i \cdot (p_i - eA_i) + m\sigma^z) f_{\alpha} \]

\[ + \sum (f_{0}^\dagger \Delta \sigma^0 f_{1} + h.c) - \frac{\Delta^2}{V} \]  
(5.6)

In this form, the QPT between QAH and QSH phases is not obvious. To clarify the physics, we use the matrix forms of this Hamiltonian

\[ H = F^\dagger H F - \frac{\Delta^2}{V} \text{ as in the QAH case.} \]  
(5.7)

The first observation is that the spectrum of the Hamiltonian is always non-degenerate. Moreover, because \( \sigma^z \tau^0 \) commutes with \( \sigma^0 \tau^x \), we have masses \( m - \Delta \) and \( m + \Delta \) for the Dirac fermions. Explicitly, the spectrum is

\[ E(p, r, s) = sgn(s) \sqrt{p^2 + (m - sgn(r)\Delta)^2}, \quad s, r = \pm 1 \]  
(5.8)

Note that one of the masses changes its sign at \( m = \Delta \), thus there is a QPT. Except at the QPT point, we have a fully gapped spectrum. Upon changing the sign of the mass, the system could change its chirality. To see that it does, we do a unitary transform to get a block-diagonal form of (5.7):

\[ H = \begin{pmatrix} m & p_+ & \Delta & 0 \\ p_- & -m & 0 & \Delta \\ \Delta & 0 & m & -p_+ \\ 0 & \Delta & -p_- & -m \end{pmatrix} \]  
(5.9)

From this representation, it is clear that we have a QPT at \( m = \Delta \) as there is an abrupt change in the winding numbers at \( m = \Delta \). Each block has the winding number \( sgn(m + \Delta)^{\frac{1}{2}} \) and \( sgn(m - \Delta)^{\frac{1}{2}} \). For \(|\Delta| > |m|\), we have two cones of different chirality and thus we are in QSH. However, if we pass through \(|\Delta| < |m|\), we have two cones of the same chirality and thus we are in QAH (See Fig.5.2).

Note that our QSH phase does not support the helical edge state at the boundary of the sample (however, see the appendix [11] though the quasiparticles in the bulk low-energy theory can be considered in the standard QSH or two-dimensional topological band insulator phase. When the higher order kinetic energy correction to the Dirac Hamiltonian is included (e.g the hexagonal warping term \( \sim \lambda(k^3 + k^3)\sigma^z\)), the winding numbers for QSH phase are changed from \( \pm 1/2 \) to zero for the both Dirac sectors. However, the low energy theory of our QSH phase is the same as that of the standard QSH physics.
In this section, we have seen from the band structure of the Hamiltonian (5.1) that there is a QPT between QSH and QAH phases. The QPT is driven by the competition of magnetic mass \( m \) (which prefers the QAH phase) and exciton mass \( \Delta \) (which prefers the QSH phase). At the transition, the mass gap vanishes and there is a change of the band structure’s chirality. Except at the transition point, we always have a gap for the single-particle spectrum. The goal of the next section is to obtain the key universal properties of the two phases in an abstract approach that is less dependent on microscopic details.
5.2 Effective theory for vortices and fluctuations

Now that we have identified the chirality and chern numbers, we integrate out the fermions to obtain effective descriptions for the fluctuations and vortices of the order parameters and gauge fields. First, we identify which fields and vortices might appear in the effective theory. To do this, we include all possible interactions and write them as gauge fields acting on the Dirac fermions. We also include $L_{\text{kin}}(\Delta)$, the kinetic term for $\Delta$.

\[
H = \sum_{\alpha} f_{\alpha}^\dagger ((-1)^\alpha \sigma^i \cdot (p_i - eA_i^\alpha) + m\sigma^z) f_{\alpha} + \sum (f_{\alpha}^\dagger \Delta \sigma^0 f_{\alpha} + h.c) + L_{\text{kin}}(\Delta) \tag{5.10}
\]

Here, $A_i^\alpha$ is the electromagnetic gauge field of the layer $\alpha = 1, 2$. From the gauge fields $A_1^1$ and $A_2^2$, we can define $A = A_1^1 + A_2^2$ which couples to the total electromagnetic charge and $\beta = (A_1^1 - A_2^2)/2$ which couples to axial charge. Before getting into the details of the effective field theory, we study the nature of the vortex in the condensate. Especially, whether the vortex is accompanied with the gauge flux or not is crucial for the properties of the vortex. So, we begin with the kinetic term $L_{\text{kin}}(\Delta)$ for the exciton condensate. Due to the gauge symmetry of the exciton order parameter $\Delta = \langle f_1^\dagger \sigma_1 f_2^\dagger \sigma_2 \rangle$, the axial gauge $\beta_\mu$ couples to $\Delta$ minimally

\[
L_{\text{kin}}(\Delta e^{i\phi}) \approx |\Delta|^2 U^{-1} |\partial_\mu \phi - 2\beta_\mu|^2 = \frac{\rho_s}{2} |\partial_\mu \phi - 2\beta_\mu|^2 \tag{5.11}
\]

which is XY - model (of the phase stiffness $\rho_s = |\Delta|^2 / U$) coupled to the gauge field $\beta_\mu$. Now, we imagine the vortex configuration of $\beta_\mu$ which can be generated by the solenoids placed near to the exciton condensate (Fig.5.3). The similar experimental scheme has been considered in the papers[127,128]. Then, the standard dual transformation allows us to write $\partial_\mu \phi - 2\beta_\mu \to 0$ for the vortex configuration of the exciton condensate. Hence, $\tilde{\beta} = \pi Z$ for the vortex in the condensate. This duality can be readily seen if we do the particle-hole transformation of the exciton order parameter $\Delta = \langle f_1^{1\dagger} f_2^2 \rangle$ for the layer 2 only. Upon the particle-hole transformation of the layer 2, we see the exciton order $\Delta$ becomes the superconducting order parameter $(\Delta \to \langle f_1^{1\dagger} f_2^{2\dagger} \rangle)$. Thus, the exciton condensate is a ‘superconductor’ in the axial channel and an insulator in the total charge channel as noted before[127]. Here, if we have an axial vortex configuration for $\beta_\mu$, we have the counterflow (or an axial current) $J_{cf} \sim \rho_s \partial_\mu \phi$ encircling the vortex to screen the phase gradient due to $\beta_\mu$ (or vice versa). We estimate the screening length by

\[
L_{\text{kin}} = \frac{\rho_s}{2} |\partial_\mu \phi - 2\beta_\mu|^2 + \frac{1}{2e^2} (\partial \beta)^2 + \frac{1}{4e^2} (\partial A)^2 \tag{5.12}
\]

where the last two terms are the kinetic energy for the gauge $\beta$ and $A$ which is obtained from the maxwell term for $A_\mu^1 (= \beta_\mu + A_\mu / 2)$ and $A_\nu^2 (= \beta_\nu - A_\nu / 2)$. Hence, we identify an axial screening length $\lambda_s \sim 1/\sqrt{\rho_s e^2}$. Note that there’s no screening length for total electromagnetic gauge field $A_\mu$ which reveals that we have an insulator in total charge channel.
In principle, there should be another term \( \sim (\beta \mu / ed)^2 \) in Eq. (5.12) when the film height \( d \) gets thin enough. However, we ignore this term upon assuming that the film is not too thin \( d > O(1) \). Though the energy of the vortex in the exciton superfluid could be reduced from infinity (\( \sim \log L \) of the system size \( L \)) to finite value by screening, it might be costly for the gauge field \( \beta \mu \) for the vortex configuration. We will compare the energy cost for the gauge configuration of the screened vortex with the energy of the unscreened vortex and see when the vortex will tend to be screened by \( \beta \mu \). To do so, we roughly estimate the energy cost for the magnetic field configuration \( \text{spontaneously} \) driven (without the externally imposed magnetic fields in the condensate) by the screened vortex \( \Phi = \pi \). We imagine that the magnetic field is dragged from infinity to the center of the circular exciton condensate of radius \( L \) (with height \( d \)) and pulled out through the vortex positioned at the center of the condensate (See figures B. and C. of Fig. 5.3). Magnetic field configuration \( \vec{B}(r) = B(r) \hat{e}_r \) is

\[
B(r) = \frac{\Phi_0}{2\pi r \cdot d}
\]

with the unit vorticity \( \Phi_0 \). The electromagnetic energy for this configuration \( \int \frac{1}{2} \chi_e B^2 \) grows as \( \chi_e \Phi_0^2 \log L \). Hence, if we compare the energy \( \sim \rho_s \Phi_0^2 \log L \) of the unscreened vortex and the energy \( \sim \chi_e \Phi_0^2 \log L \) of the screened vortex, we conclude to have screened vortices if the magnetic permeability of the exciton condensate \( \chi_e \) is much smaller than the phase stiffness \( \rho_s \). When this is not the case, there could be more interesting possibilities such as the irrational charge and statistics for vortices. We refer the reader for this discussion to the paper [123] and the references there-in. On the other hand, if the magnetic field is supplied by the external mean such as the experimental set-up in our scheme (Fig. 5.3) or Fig.1 of the papers [127, 128], it is much easier for the condensate to have the screened vortices. The vortex in the condensate can save logarithmically divergent energy cost (\( \sim \log L \)) by slightly tilting and trapping the magnetic fluxes which should take finite energy, and this concludes that the vortex in our experimental scheme will be always accompanied with the gauge flux \( \Phi = \pi Z \) (Fig. 5.3).

Another comment is in order. Even though the exciton order parameter \( \Delta \) in the mean field theory is of the same form to the tunneling term between layers, tunneling term introduces a new term to the effective field theory \( L_{\text{tun}} \sim -t \cos(\phi) \) as it tends to pin down the \( U(1) \) phase of the exciton order parameter (\( t \) is proportional to the tunneling strength between layers). This term breaks \( U(1) \) symmetry and induces ‘sine-Gordon’ theory coupled to the vortex matter which can be ignored as \( t \to 0 \) in our perspective [129].

Now that the allowed gauge couplings are identified, the fermions are integrated out to obtain the effective theory which is the main result of this section:

\[
L = \text{sgn}(m + \Delta) \frac{\varepsilon^{\mu\nu\lambda}}{8\pi} (A + \beta)_\mu \partial_\nu (A + \beta)_\lambda + \text{sgn}(m - \Delta) \frac{\varepsilon^{\mu\nu\lambda}}{8\pi} (A - \beta)_\mu \partial_\nu (A - \beta)_\lambda + O((\partial A)^2) \tag{5.14}
\]
Figure 5.3: Illustration of the generating axial gauge fluxes. General idea is to make magnetic field configuration which has $\int (B_1^1 - B_2^2)$ nonzero. A. Experimental scheme similar to that of the paper[127]. We place magnets or solenoids at the boundary of the sample. B. Experimental scheme similar to that of the paper[128]. We place solenoids on the top and below of the condensate. Without the solenoids, the vortex should create the magnetic flux itself to be screened. To estimate the energy of the vortex roughly (see the text), we consider that the flux enters at the vortex and leaves at the boundary of the sample. C. Top view of the scheme B. The exciton condensate has the radius $L$, and the solenoids are placed at the center of the condensate.
Section 5.2. Effective theory for vortices and fluctuations

(with $e = 1$). Here, we ignore the Maxwell term as the Chern-Simons (CS) term dominates the low energy physics. The appearance of the doubled CS theory is due to the two massive Dirac cones in Eq. (5.7) where we gauge one Dirac cone of mass $(m + \Delta)$ with $A_\mu + \beta_\mu$ and the other Dirac cone of mass $(m - \Delta)$ with $A_\mu - \beta_\mu$ and integrate out those gapped fermions to obtain the gauge theory of $\beta_\mu$ and $A_\mu$. This phenomenological approach reproduces the essential feature of Eq. (5.14) which is consistent with the previous study [123]. We will also justify this effective theory Eq. (5.14) in the later part of this section. However, readers interested in a more detailed derivation of Eq. (5.15) and Eq. (5.18) from the Dirac hamiltonian are referred to the paper [123] where this field theory is rigorously considered. In this field theory, we observe the coefficient of the CS term for $A$ changes at $m = \pm \Delta$. This signals the QPT at $m = \pm \Delta$. This simple theory captures nearly every essential property of the vortices and fluctuations of the system; the rich behavior of the vortices includes localized charges.

For the QSH phase ($|\Delta| > |m|$), we have (up to the sign factor infront of the mutual CS theory for $\beta_\mu$ and $A_\nu$)

$$L = \frac{1}{2\pi} \varepsilon^{\mu\nu\lambda} \beta_\mu \partial_\nu A_\lambda + O(\partial A)^2$$

(5.15)

From this effective mutual CS (or equivalently $BF$) theory for $\beta_\mu$ and $A_\nu$, we can directly read off charge and statistics information for the exciton vortices. Here, it is interesting to notice that $BF$ theory emerges for QSH phase which reflects the time reversal symmetric nature of the phase. We now study the charge and statistics of the vortices. First, we see that the absence of the topological term for $\beta$ requires that the vortices have no statistics (statistical angle $\theta = 0$). However, the EM charge localized at the vortices is non-trivial in that $q = \int \frac{4L}{\beta A} = \int \frac{1}{2\pi} \partial \beta = \frac{1}{2\pi} \int \beta = \pm 1/2$, that is, we have a half of electron charge localized at the vortex, which is consistent with the previous consideration on the vortices of TEC ($\Delta = 0$). In comparison with the paper [123] and our result Eq. (5.15), we note that we miss the coefficient $sgn(\mu_s)$ for $BF$ term which matters for the sign of the fractional charge at the vortex but this sign factor is not important for our thin film topological insulator problem. The electric charge of the fermionic zero mode at TEC is known to be defined modular integer [121] in connection with the axionic $\theta$-vacuum i.e., the localized charge at the vortex is $-e(1/2 + n)$ for $n \in \mathbb{Z}$, and thus the sign of the fractional charge (or the sign of $BF$ term in Eq. (5.15)) shouldn’t be taken seriously. As was noticed in the earlier study of the fractional charge, the $\pm e/2$ charge is associated with the zero mode solution for the vortex. Therefore, we look for the solution of $H \Psi = 0$ such that

$$H = \begin{pmatrix}
  m & (p_+ - A_+) & \Delta e^{-i\theta} & 0 \\
  (p_- - A_-) & -m & 0 & \Delta e^{-i\theta} \\
  \Delta e^{i\theta} & 0 & m & -(p_+ - A_+) \\
  0 & \Delta e^{i\theta} & -(p_- - A_-) & -m
\end{pmatrix}$$

(5.16)

which is the Hamiltonian for the exciton vortex with vorticity $-1$. We solve this problem by the following ansatz $\Psi \sim (u_1, v_1, v_2, u_2)^T$ with the constraint $u_1^* = -u_2$ and $v_1^* = v_2$ [121, 127].
Then, the single phase method provides $u_1 \sim u_2^* \sim e^{-i\theta} \text{ and } v_1, v_2 \text{ independent of the angular variable } \theta$. With this in mind, we use the following ansatz

$$
\begin{align*}
  u_1(r, \theta) &= f(r)e^{i\pi/4} e^{-\int r' \Delta(r') dr'} e^{-i\theta}, \\
  v_1(r, \theta) &= g(r)e^{-i\pi/4} e^{-\int r' \Delta(r') dr'}
\end{align*}
$$

Upon substituting this ansatz, it is straightforward to solve the resulting differential equation and the solution is $u_1 \sim \exp(-\int r' \Delta(r') dr') I_0(mr)$ and $v_1 \sim \exp(-\int r' \Delta(r') dr') I_1(mr)$ where $I_n$ is the $n$th modified Bessel function. This wavefunction is convergent if and only if we are in QSH phase $|m| < |\Delta|$.

The statistical phase and localized charge of the vortex can be understood by the following adiabatic argument. In the QSH phase, we have two gapped Dirac fermions and they carry half-filled quantum Hall effect with the opposite chirality. When we thread the axial flux $\beta = \pi$ adiabatically to the system which is identical to an exciton vortex of the circulation $2\pi$, each quantum Hall state collects charge $e/4$. Thus, the localized charge of the vortex is $e/2$ ($= e/4 + e/4$). When we do the pair-wise exchange of the vortices, the statistical phase accumulated is $0$ ($= \pi/8 - \pi/8$) because the statistical phase $\pi/8$ from one quantum hall state is precisely cancelled by the phase $-\pi/8$ from the other. Hence, the vortex in the QSH phase has no statistical angle: $\theta = 0$.

In terms of the external EM gauge $A$, we have the response $\sim O(\partial A)^2$ which is the Maxwell kinetic term and non-topological. However, the topological property shows up in principle if we consider a particular type of the domain wall for the exciton mass $\Delta$. (Appendix)

For the QAH phase ($|\Delta| < |m|$), we have

$$
L = \frac{1}{4\pi} \epsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda + \frac{1}{4\pi} \epsilon^{\mu\nu\lambda} \beta_\mu \partial_\nu \beta_\lambda + O(\partial A)^2
$$

From this effective theory, we now notice that we are in the quantized QAH from the leading CS term for the response of $A$. This tells us that we will have a circulating chiral edge state supporting the Hall conductance $e^2 / h$ at the boundary of the sample.

On the other hand, we have no crossing term between $A$ and $\beta$ implying that the vortices of the exciton order will not carry any EM charge. On the other hand, the exciton vortices is ‘anyonic’. It looks like the coefficient of CS term implies that the vortices are fermionic, but this is not the case as we have $\beta = \pm \pi \mathbb{Z}$ (In the usual CS theory $L = \frac{K}{4\pi} a \partial a$, $\beta a = 2\pi$ defines the unit vortex). With this consideration, we now have fractional statistics between vortices with the statistical angle $\theta = \pi/4$ (half of semionic statistics). Note that the vortex in QAH phase does not carry a zero mode solution for the equation (5.16). However, we can still talk about the exciton vortex as it is quantized to have circulation $2\pi \mathbb{Z}$ and well-defined excitation. This anyonic vortex emergent in QAH phase can be considered as an example of anyons from ‘weakly’ interacting systems and this is similar to the previous study on integer quantum hall effect with the fully filled lowest landau level adjacent to the type-II superconducting film.
The behavior of the vortex can be understood in terms of the adiabatic argument as before. In the QAH phase, the two sectors of gapped Dirac fermions have the same chirality. Thus, the axial gauge flux $\mathcal{A} \beta = \pi$ associated with an exciton vortex will collect $e/4$ in one sector and $-e/4$ in the other. This gives the total charge $0$ ($= e/4 - e/4$). If we exchange a pair of vortices, we now have the statistical phase $\pi/4$ ($= \pi/8 + \pi/8$) by adding up the phases accumulated from the two sectors.

We now take a different point of view to present the justification of our theory Eq. (5.14). We base on the adiabatic argument and physical understanding of the fractional charge and statistics of vortices. First, we expect that there could be (at most) two CS terms for the effective field theory of $\beta_\mu$ (axial gauge) and $A_\mu$ (electromagnetic gauge) due to the two massive Dirac cones

$$L_{\text{eff}} = \frac{C_1}{2\pi} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu \beta_\lambda + \frac{C_2}{4\pi} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda + \frac{C_3}{4\pi} \varepsilon^{\mu\nu\lambda} \beta_\mu \partial_\nu \beta_\lambda$$

(5.19)

and the effective field theory should behave well because of the gap except the critical point, i.e., the coefficients $(C_1, C_2, C_3)$ in Eq. (5.19) change only at the critical point $m = \Delta$. So our basic strategy is to extract the coefficients for QSH and QAH phases. As $T$-symmetry has the important role, we study the transformation of $\beta_\mu$ and $A_\mu$ under $T$-symmetry operation: $(\beta_0, \beta_i) \rightarrow (-\beta_0, \beta_i)$ and $(A_0, A_i) \rightarrow (A_0, -A_i)$. Thus, the first $BF$ term in Eq. (5.19) between $\beta_\mu$ and $A_\mu$ is $T$-symmetric, and the other two CS terms are $T$-breaking.

For QSH phase, the phase should respect $T$-symmetry in the effective field theory Eq. (5.19) though we break $T$-symmetry microscopically by inclusion of magnetization mass $\sim m \sigma^z$. We can extract the coefficient $(C_1, C_2, C_3)$ for Eq. (5.19) at $m = 0$ with the fixed $\Delta$ because the QSH phase with finite $|m| < |\Delta|$ is adiabatically connected to the system of $m = 0$ without closing the gap. This consideration gives $C_2 = C_3 = 0$ for the entire range of QSH phase. And we supplement the field theory with the information that the vortex $\mathcal{A} \beta_\mu = \pi$ carries the fractional charge $\pm e/2$ with finite $\Delta$ at $m \rightarrow 0$[121]. This translates to the field theory as $C_1 = 1$. Hence, we have the effective field theory for QSH phase $L_{\text{eff}} = \frac{1}{4\pi} \beta \partial A$ (with the implicit antisymmetrization of indices for fields) and this is precisely the same as the effective theory we obtained before Eq. (5.15).

On the other hand, QAH phase has the total Chern number which fixes $C_2 = 1$. For $C_1$ and $C_3$, we utilize the adiabatic argument with $\Delta \rightarrow 0$ while keeping $m$ finite. At this limit, the axial gauge flux $\mathcal{A} \beta = \pi$ associated with an exciton vortex will collect $e/4$ in one layer and $-e/4$ in the other. This gives the total charge $0$ for the vortex which translates $C_1 = 0$ for the effective field theory Eq. (5.19). When we do a pair-wise exchange of vortices $\mathcal{A} \beta = \pi$, we now have the statistical phase $\pi/4$ ($= \pi/8 + \pi/8$) by adding up the phases accumulated from the two layers. This fixes $C_3 = 1$. As a whole, we obtain the effective field theory for QAH phase $L = \frac{1}{4\pi} A \partial A + \frac{1}{4\pi} \beta \partial \beta$ (with the implicit antisymmetrization of indices for fields) which is the same as in Eq. (5.18). Finally, it is straightforward to rewrite these field theories in both phase into a single theory of the form Eq. (5.14).

In the paper[127], it is shown that the excitonic vortex may carry the irrational statistics due to the irrational axial charge $\delta Q_v = Q^1 - Q^2$ bound to the vortex. (Note that in the
Section 5.2. Effective theory for vortices and fluctuations

bilayer system, the fluctuation in the axial charge could be finite unlike the total charge which is suppressed by the Coulomb interaction between layers) With this additional axial charge and the axial \( \pi \) flux of the vortex, the statistical angle is given as \( \pi \delta Q_v \) which could be continuously tuned\[127\]. In our case, this might not be the case. First of all, there’s no term breaking the symmetry between layers (such as the voltage drops \( \mu_s \)), we don’t have any irrational statistics as the axial charge is \( \delta Q_v = 0 \) due to the symmetry between up and down layers. We also can deduce the form of the effective field theory from the adiabatic argument when the voltage drop \( \mu_s \) between layers is included in consideration. When the voltage drop \( \mu_s \) is slowly turned on from 0 in the system, we evolve the mass \( \Delta \) in Eq.\( 5.15 \) and Eq.\( 5.18 \) into \( \sqrt{\Delta^2 + \mu_s^2} \) without closing gaps (the total masses for the two Dirac cones are \( m \pm \sqrt{\Delta^2 + \mu_s^2} \)). So we predict at least in our effective field theory and the adiabatic argument that the statistics and charge of vortices are fractionalized and quantized as in the case without \( \mu_s \).

In the QAH phase, the system acquires a topological QAH response to the external EM gauge. This has a direct implication on the Faraday angle \( \theta_F \) which is related to Hall conductance \( \sigma_{xy} \) of the system\[13\] \[132\] \[134\]. In QAH phase, we expect to have a strong Faraday effect as \( T \)-symmetry is broken. On the other hand, we wouldn’t have a strong Faraday effect in QSH phase as we do not break \( T \)-symmetry effectively though we break \( T \)-symmetry microscopically. This optical response could be used in experiment to distinguish the two phases. In a thin film with interlayer coherence (exciton order), the electron tends to be ambiguous on its layer index. Thus, we can think of the thin film as like a single layer with two Dirac cones. Then, as pointed out from the previous section, we have two Dirac cones with masses \( m + \Delta \) and \( m - \Delta \), and the two Dirac cones contribute to total \( \sigma_{xy} \) equally.

We specialize for low frequency \( \omega \ll E_c \) (\( E_c \) is the cut-off for the energy, and typically we can take \( E_c \) as the bulk gap\[132\]) and the chemical potential lying in the gap. Then, at the leading order \( O(\omega/E_c, m/E_c, \Delta/E_c) \)

\[
\sigma_{xx} = 0, \quad \sigma_{xy} = \sigma_{xy}^+ + \sigma_{xy}^- \tag{5.20}
\]

where \( \sigma_{xy}^\pm = \text{sgn}(m \pm \Delta) \times \frac{\alpha}{4\pi} \left( 1 - \frac{|m \pm \Delta|}{E_c} \right) \) (Here, \( \alpha \) in the coefficient is the fine constant, i.e \( \alpha = 1/137 \)). For convenience, we take the Zeeman mass \( m \) and exciton order parameter \( \Delta \) positive. In the QAH phase, we have \( \sigma_{xy} = \alpha/2\pi \) with the limit \( m/E_c \to 0 \). This gives \( \theta_F = \tan^{-1} \left( \frac{2\alpha}{\sqrt{\epsilon_{xx}^L/\mu_c^L} + \sqrt{\epsilon_{xx}^R/\mu_c^R}} \right) \sim 10^{-3} \) rad, which is simply the double of the previously studied on the single-layer Dirac cone with \( T \)-breaking. In the QSH phase, where we preserve \( T \)-symmetry effectively, we have totally different behavior in that \( \sigma_{xy} = \frac{\alpha}{4\pi} \times \frac{2m}{E_c} \to 0 \) in the limit \( m/E_c \to 0 \). Thus, there is no significant \( \theta_F \) even though \( T \)-symmetry is broken at a microscopic level. The small \( T \)-breaking shows up only in the order of \( O(m/E_c) \); \( \theta_F \sim \alpha \times O(m/E_c) \). If we plug \( m \sim 10 \text{ meV} \) and \( E_c \sim 0.3 \text{ eV} \) for Bi\(_2\)Se\(_3\), then we have \( \theta_F \sim \alpha \times O(m/E_c) < 10^{-4} \) rad, much smaller than \( \theta_F \) for QAH phase.
5.3 Uniform orbital magnetic fields in a thin film

We have seen that the interplay between Zeeman and exciton masses induces interesting physics on the vortices and in the electromagnetic response. However, there is another natural way to break the $T$-symmetry: uniform magnetic fields along $\hat{z}$. We have Zeeman interaction due to magnetic field $B$ via $\sim g\sigma_z B$ but we also have Landau Levels (LL). We will see that the zeroth LL will determine the physics and we can obtain the same effective theory as before. The appearance of the same effective theory can be traced back to the CS effective theory for QHE. Now, the coefficient of the effective theory is decided by the filling of the LLs, rather than the winding numbers of the band structures, and the phase transition at $m = \Delta$ is replaced by the quantum hall phase transition where the filling of LLs are suddenly changed. We begin with LLs of Dirac fermions which is similar to graphene. But the crucial difference here is the Zeeman coupling and degeneracy. Under the uniform magnetic field $B$, electrons form the LLs with index $N \in \mathbb{Z}$

$$E(N, r) = sgn(N)|v_F|\sqrt{C}|N| + (m + sgn(r)\Delta)^2$$

$$r = \pm 1, N \neq 0$$

and $C = \frac{e\hbar B_z}{\pi e}$. The zeroth LL is sensitive to the competition between $m$ and $\Delta$ in that (See also Fig. 5.4)

$$E(N = 0, r) = m + sgn(r)\Delta, \quad r = \pm 1$$

We begin with the case where the chemical potential lies at $E_F = 0$ as before. Then, we see that every LL with negative (positive) index $N$ is always filled (empty) independent of the parameters $B, m$ and $\Delta$. However, the filling of the zeroth LL is dependent of the parameters (See Fig. 5.4). For $m > \Delta$, we have that both of zeroth LLs are empty (as they are above the chemical potential $\mu = 0$). Thus, we have QHE with the quantized hall conductance $\frac{e^2}{h}$ (Note that there is an offset by 1/2 of the QHE for Dirac fermions). On the other hand, if we have $m < \Delta$, one LL is filled and the other is empty so we have a spin-Hall-like response. For the QHE, CS theory is the effective field theory

$$L_{QHE} = \frac{1}{4\pi K} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda$$

(5.23)

where $K$ is the inverse of the filling (i.e $K = 1/\nu$). Hence, we conclude the effective theory for the system as $K = \pm 2$ (The sign of $K$ is determined by $m$ and $\Delta$)

$$L_{QHE} = sgn(m - \Delta)\frac{\varepsilon^{\mu\nu\lambda}}{8\pi} A_{1\mu} \partial_\nu A_{1\lambda}$$

$$+ sgn(m + \Delta)\frac{\varepsilon^{\mu\nu\lambda}}{8\pi} A_{2\mu} \partial_\nu A_{2\lambda} + O((\partial A)^2)$$

(5.24)

This is exactly the same effective field theory before (5.14), and what all we need to do is to assign the correct coupling of axial gauge $\beta$ for each of the zeroth LLs. The two LLs are
from the two Dirac cones of the opposite axial charge $\pm 1$ and the same EM charge $+1$, i.e., $A_1 = A + \beta$ and $A_2 = A - \beta$. Upon plugging this in, we restore the same effective field theory Eq. (5.14) as in the previous section. Thus, we have the same charges and statistics if we include the vortex fields in the effective theory. We see immediately that much of the physics studied in the previous section applies in this case.

However, the zero energy solution for the magnetic field case is not trivial to generalize as the uniform magnetic field cannot be gauged away. Furthermore, this uniform orbital magnetic field destroys the particle-hole symmetry of the Hamiltonian, and thus we cannot use the same ansatz Eq. (5.17) with $\Psi \sim (u_1, v_1, u_2, v_2)^T$ and $u_1^* = -u_2$ and $v_1^* = v_2$. This form of the ansatz relies on the anticommutation relation $\{C, H\} = 0$ where $C = i\tau^y\sigma^yK$ and $K$ is the complex conjugation. With the orbital magnetic field, we no longer have the anticommutation relation $\{C, H\} \neq 0$. This manifests in the LL spectrum (See Fig. 5.4). So we instead make an ‘educated guess’ for the ansatz $\Psi \sim (u_+, v_+, v_-, -u_-)^T$ and

$$u_\pm(r, \theta) = f_\pm(r)e^{\pm i\pi/4}e^{-\int^r \Delta(r')dr'}e^{-i\theta},$$
$$v_\pm(r, \theta) = g_\pm(r)e^{\pm i\pi/4}e^{-\int^r \Delta(r')dr'} (5.25)$$

With this ansatz, we obtain four independent linear equations of $f_\pm(r)$ and $g_\pm(r)$

$$mf_+ + \Delta g_+ + \left(\frac{\partial}{\partial r} + \frac{Br}{2}\right)g_+ = 0$$
$$mg_+ + \Delta f_+ + \left(\frac{\partial}{\partial r} + \frac{1}{r} - \frac{Br}{2}\right)f_+ = 0$$
$$mg_- + \Delta f_- + \left(\frac{\partial}{\partial r} + \frac{1}{r} + \frac{Br}{2}\right)f_- = 0$$
$$mf_- + \Delta g_- + \left(\frac{\partial}{\partial r} - \frac{Br}{2}\right)g_- = 0 (5.26)$$

We can try to solve this system of differential equations by reducing into the following two equations via canceling $f_-$ and $g_-$ in the above equations.

$$(M^2 + \partial^2 + \frac{2}{r}\partial - \frac{B}{2} - \frac{B^2r^2}{4})f_+ + m(2\partial + \frac{1}{r} + Br)g_+ = 0$$
$$(M^2 + \partial^2 + \frac{B}{2} - \frac{B^2r^2}{4})g_+ + m(2\partial + \frac{1}{r} - Br)f_+ = 0 (5.27)$$

where we abbreviate $\frac{\partial}{\partial r} = \partial$ and $M^2 = m^2 - \Delta^2$. The above differential equation Eq. (5.27) is difficult to solve and not clear if they admit analytic solutions without approximations. Rather than directly attempting to solve the system of differential equations, we look for a few solvable limits with the analytic solutions in terms of the confluent hypergeometric functions. The most convenient and important limit is when the zeeman coupling vanishes ($m \to 0$) which effectively decouples $f_\pm$ and $g_\pm$. In this limit, the solution for Eq. (5.27) is
Figure 5.4: Illustration of the Landau Levels depending on the parameter $m > 0$ and $\Delta > 0$. Here, we assumed $\Delta \neq 0$. We always keep the chemical potential $\mu$ at $E = 0$, and the 0th LL passes through the fermi energy $E = 0$ at $m = \Delta$. The levels of LL index $n$ with $n \neq 0$ never change their filling as their energies are always positive (if $n > 0$) or negative (if $n < 0$). These levels (blue) do not play an important role. On the other hand, the two 0th LLs drive the quantum phase transition at $m = \Delta$ because the sign of their energies are dependent on $m$ and $\Delta$. The filling of the lower 0th LL (red) in the figure is abruptly changed at $m = \Delta$ as it passes through $\mu$. A. the LLs of the case $\Delta < m$. The lower 0th LL is fully- filled B. when $\Delta = m$, the 0th LL experiences change in its LL filling. C. Passing $\Delta > m$, the 0th LL is fully emptied.
Section 5.4. Conclusion

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\[ f_\pm = 0 \text{ and } \]

\[ g_+(r) \sim \frac{1}{\sqrt{r}} W\left(\frac{1}{4} - \frac{\Delta^2}{2B}; -\frac{1}{4}; \frac{Br^2}{2}\right) \]  

(5.28)

where \( W\left(\frac{1}{4} - \frac{\Delta^2}{2B}; -\frac{1}{4}; \frac{Br^2}{2}\right) \) is the Whittaker function\(^{[135]}\), or equivalently we can represent it as the parabolic cylinder function \( g_+(r) \sim D_p\left(\frac{Br^2}{2}\right) \) with \( p = -\frac{\Delta^2}{2B} \) which appears in the Kekule vortex solution in the graphene\(^{[124]}\) under the uniform orbital magnetic field. This limit of the solution corresponds to the case \(|\Delta| >> |m|\), i.e., the negligible zeeman coupling.

The other important limit where we can obtain an analytic solution for Eq. (5.26) is when \( r \to \infty \). In this limit, we ignore the potential terms of the order \( \sim O(1/r) \) for \( f_\pm \) and \( g_\pm \) in Eq. (5.26). From this approximation, we try to see if there’s a convergent solution for the system of differential equations. In the limit \( r \to \infty \), we obtain

\[ g_+(r) \sim \frac{1}{\sqrt{r}} \left\{ C_1 W\left(\frac{1}{4} - \frac{(\Delta - m)^2}{2B}; -\frac{1}{4}; \frac{Br^2}{2}\right) + C_2 W\left(\frac{1}{4} - \frac{(\Delta + m)^2}{2B}; -\frac{1}{4}; \frac{Br^2}{2}\right) \right\} \]  

(5.29)

with the initial condition dependent coefficients \( C_1 \) and \( C_2 \). It is now obvious that the solution \( g_+(r) \) in Eq. (5.29) reduces to \( g_+(r) \) from Eq. (5.28) when \( m/|\Delta| \to 0 \). As \( g_+(r) \sim r^{2M} \exp(-Br^2/4)(1 + O(1/r^2)) \) as \( r \to \infty \) where \( M = (m + \Delta)^2 \), the ignored potential term \( \sim O(1/r) \) in Eq. (5.26) will not generate more singular terms than \( r^{2M} \exp(-Br^2/4) \) in power series expansion near \( r \to \infty \). Note that the exciton vortex in the uniform orbital magnetic case carries the same charge and statistics as the case without the orbital field due to the same form of the effective topological field theory despite of the different forms for the zero mode solutions.

5.4 Conclusion

In summary, we have studied a thin film of topological insulator with both \( T \)-breaking Zeeman mass and \( T \)-symmetric excitonic mass. The two masses compete with each other and result in two topologically distinct phases for the elementary excitations: quantum anomalous Hall (QAH) and quantum spin Hall (QSH). We studied the effective theory for the electromagnetism and exciton order parameter vortices by integrating out the fermions, and there can be other topological properties such as a helical metal at a particular kind of domain wall of the exciton order parameter. We also obtained explicit wave functions for the fermion zero mode at the vortices. There is one zero mode for QSH and no mode in the QAH regime, and found the zero mode solution under a uniform magnetic field in some limits.

Before finishing this paper, we would like to emphasize some relevant facts for practical observation of exciton condensation in a topological insulator (TI) thin film. In principle, TI might host a higher transition temperature \( T^* \) for the exciton superfluid-insulator transition
than graphene, resulting from the decreased number of fermion flavors. In graphene, there has been intense theoretical study of the exciton condensates, and the estimated transition temperature for graphene ranges from milliKelvin\[136\] to room temperature\[137\]. An important reduction comes from the large number of fermion species in the screening\[136\] ($N = 8$ for bilayer graphene) which induces the factor $T^* \sim e^{-16}E_f$ where $E_f$ is the fermi energy of the system even though the bare interaction energy scale (without screening) is not small $r_s = e^2/\epsilon v_f \sim 1$ in the graphene. However, the thin-film topological insulator contains only two species $N = 2$ because we have only one Dirac fermion per layer. But we have the disadvantageous situation for $r_s$ as in many current materials the dielectric $\epsilon$ for TIs are quite large (ranging from 30 to 80) though $v_f \sim 10^5 m/s$ which is nearly half of graphene case. (An additional problem of early TI materials, that they were not in practice very insulating, seems to have been overcome.) These two factors contribute to reduced values $r_s \sim 1/3 - 1/8$. However, we can look for higher $r_s$ and thus higher transition temperature by noting that the main drawback comes from the large $\epsilon$ which is material-dependent; a possible solution is to sandwich a thin normal insulator of small $\epsilon^*$ between two topological insulators (See Fig.3.1 B), and which will change $r_s \rightarrow e^2/\epsilon^* v_f$ which could be as large as 3 if $\epsilon^* \sim 10$. This might open a way to achieve a dramatic increase in the superfluid transition temperature and realize the surprising physics of the topological exciton condensate.

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Part II

Beyond topological band insulator
Chapter 6

Dyon condensation in topological Mott insulators

6.1 Introduction to topological Mott insulator

One of the most notable progresses in modern condensed matter physics is the development of the concept of “topological order”. Topologically ordered phases cannot be understood in terms of order parameters, which are the bases of Landau-Ginzburg theories of broken-symmetry phases. Standard examples of the topological order include quantum Hall phases\cite{1,64} and time-reversal symmetric topological insulators\cite{5–8,83} (we will abbreviate ‘time-reversal symmetric topological insulator’ as ‘topological insulator’). Topological insulators are insulating in bulk but have gapless edge or surface states which are ‘immune’ to the opening up of a gap as long as the time-reversal symmetry is respected. Though the protected gapless edge/surface state itself is quite interesting, it is notable that the topological band insulator can provide a condensed-matter example of axionic electromagnetism\cite{13–15}

\[ L_\theta = \frac{\theta}{32\pi^2} \varepsilon_{\mu\nu\lambda\rho} F_{\mu\nu} F_{\lambda\rho}, \]

(6.1)

when the surface is gapped by the time-reversal symmetry breaking perturbations. In condensed matter physics language, this axionic term can be understood as a half-integral surface quantum Hall effect\cite{13}. This quantized anomalous Hall effect and other interesting surface and bulk physics of the topological band insulator have attracted both the theoretical and experimental interest\cite{21,39,41,121,132,138,143}.

Axionic electromagnetism, especially in the presence of a dynamical gauge field, has a long history in high-energy physics. The interest in the axion term stems from the CP-violation problem\cite{144,146} and confinement of quantum chromodynamics\cite{16}. Though the axion term Eq.\cite{6.1} is a total derivative, t’Hooft et.al.\cite{16} showed that the axion term is capable of changing the nature of the instantons and the confined phases in non-abelian gauge theories. The phase where the dyon is condensed in the presence of the axion term has a qualitatively different structure from the ordinary confined phase; this difference is
traced back to the fact that the monopole receives the gauge charge due to the axion term (this effect is sometimes called “Witten effect”[147]). Similar behavior can emerge in abelian gauge theories on the lattice; Cardy et.al.[148] studied the phase diagram of the gauge theory with the axion term and demonstrated oblique confinement in the discrete \( \mathbb{Z}_p \) gauge theory and the compact \( U(1) \) gauge theory. The structure of the phase diagram and the related \( SL(2; \mathbb{Z}) \) symmetry are well studied[148–150].

As we now have a condensed matter system exhibiting axion electromagnetism, we are led to the natural question: could we find an example where the axion term changes the nature of the phases and phase transitions in the condensed matter system? The monopole in the presence of the axion term becomes a dyon with the fractional charge[16, 147, 151], and the structure of the confined phase should reflect this fractional charge of the dyon. In this paper, we will seek to find a condensed matter example of this novel confined phase which reflects the axionic electromagnetism and dyon condensation. To study the confinement, it is important to allow magnetic monopoles in the excitation spectrum. At the same time, the compactness of the \( U(1) \) gauge theory is important for the existence of monopoles. Hence, to study the confined phase with Witten effect, we need both a compact \( U(1) \) gauge theory (or non-Abelian gauge theory) and the axion term. Clearly, the usual electronic topological band insulators with the non-compact “external” electromagnetic fields cannot provide such an example. In the condensed matter system, the compact \( U(1) \) gauge theory on the lattice often emerges as a consequence of “fractionalization” of the electron. It has been suggested that the so-called topological Mott insulator, where the fractionalized excitations or spinons possess topological band structure, satisfies

There may be two different routes to obtain topological Mott insulators. First, one could start from an electronic band insulator[152]. Upon increasing the on-site Hubbard interaction, there may be a transition to a spin liquid Mott insulator. As the excitations in the spin liquid are fractionalized, such a transition can be regarded as the Bose condensation of the charge-carrying degrees of freedom such that the Bose condensed phase corresponds to the topological band insulator. On the spin liquid side, the charge degree of freedom is gapped, but the resulting fermionic spinons with spin-1/2 quantum number inherit the topological band structure of the underlying electrons. The spinons with such topological structure, in turn, couple to an emergent \( U(1) \) gauge field. When the fermionic spinons are integrated out, the non-trivial topology of the spinon spectra leads to an axion term for the emergent \( U(1) \) gauge field. In the second case, one may start from spin models[153] with frustrated antiferromagnetic and ferromagnetic exchange couplings. It was recently shown that slave-fermion theory of such spin models can support a \( U(1) \) spin liquid with an emergent spin-orbit coupling, hence the topological band structure of the spinons. In this case, the non-trivial topology of the spinon spectra is emergent and not inherited from the electrons. Similarly to the first case, the axion term would arise upon integrating out the spinons in the bulk.

In order to gain some insight as to the dyon condensate in the topological Mott insulator, we start by briefly reviewing the confined phase and the Higgs phase[154, 155], driven from a “bosonic” \( U(1) \) spin liquid by condensing the monopole and the “bosonic” spinon. The
condensation of bosonic spinons leads to the conventional Neel phase. On the other hand, we obtain the Valence Bond Solid (VBS) state if we condense the monopoles in the $U(1)$ spin liquid in $(3 + 1)$D, which can be understood as the confinement of electric fluxes. In the VBS state, we have confined spinons and no “photon”. As there are significant connections between the ordinary confined phase and the oblique confined phase, we discuss first the nature of the ordinary confined phases. First, the non-trivial spatial patterns of VBS originate from the crystal momentum carried by the monopole operators. The crystal momentum can be traced back to the nontrivial Berry phase due to the background staggered $U(1)$ gauge charge. The staggered $U(1)$ gauge charges induce the background “electric” fluxes connecting charges. When a monopole hops around the dual lattice, it sees the “electric” fluxes and feels the Aharonov-Bohm phase. This is exactly dual to the standard Aharonov-Bohm phase for electric charge circulating around magnetic flux. Due to the Berry phase for the monopole, the monopole tends to condense at a finite momentum. Condensation of a monopole at a finite momentum implies that there is a non-trivial spatial pattern of the monopole current\[154, 155\]. Then, the monopole current will induce the “electric” fluxes just like an electric current inducing a magnetic field. As the valence bond operator is proportional to the “electric” flux, we end up with patterns of valence bonds.

Some of the above discussions for the standard confined phase can be applied to the confined phase driven by dyon condensation in the topological Mott insulators. First of all, the dyon will experience a Berry phase if there is a nontrivial background charge pattern because the dyon carries both the “magnetic” and “electric” charges. It will be shown in the main text that there exists another contribution to the Berry phase due to the axion term in the topological Mott insulator. Secondly, when the dyon with a non-zero crystal momentum condenses, the system supports both the “electric” current and “magnetic” monopole current. The dyon current then will induce the ‘magnetic” fluxes as well as the “electric” flux. The “magnetic” flux should be naturally accompanied by the gauge-charge current in the oblique confined phase. Hence, we obtain a nontrivial phase where the gauge-charge current order coexists with the bond order when the dyon condenses.

There are a number of subtle issues in dyon condensation and the physical interpretation of such phenomena. First, it is known that the statistics of the dyons may not be trivial\[156–164\]. We show that there is no statistical transmutation for the dyons in the topological Mott insulator. Thus the dyons are bosons as far as the monopoles are bosonic\[157, 160\]. Secondly, we argue that the monopoles in topological Mott insulators have as their quantum numbers only the $U(1)$ gauge charge and crystal momenta. (From the discussion of the usual topological band insulator\[13, 14\], we physically understand the gauge charge of a monopole as a ‘polarization’ charge so that the dyon is not a bound ‘particle’ to the monopole. This understanding of the charge of the dyon perhaps implies that there will not be a statistical transmutation as the charge is more like a polarization ‘cloud’, not a particle). The actual pattern of the dyon condensate depend on the details of the microscopic physics, i.e., the lattice structure and the background charges. In this work, we discuss the dyon condensation patterns and their physical implications on the cubic lattice.

The rest of the paper is organized as follows. In section II, the field theory of dyons on
the dual space/lattice is derived starting from the U(1) gauge theory with axion term on the
direct space/lattice. We discuss possible dyon condensation patterns and resulting confined
phases in section III. We summarize our results and conclude in section IV.

6.2 The field theory of dyons on the dual lattice

We consider fermionic spinons on a cubic lattice for simplicity to develop the basic idea
of dyon condensation. In the following section we connect the general considerations in this
section to possible phases proximate to the topological Mott insulator state.

In order to derive the action for the dyons (or monopoles), we first need to integrate
out the gapped matter fields in the system and obtain an effective gauge theory. As the
fermionic spinons are in the topological insulator state, the topological nature of the spinon
states leads to an axion term in the effective $U(1)$ gauge theory as follows:

$$L_A = L_{QED} + L_\theta$$

(6.2)

The first term $L_{QED}$ describes lattice quantum electrodynamics in $(3+1)$D in the presence
of the staggered gauge charge

$$L_{QED} = \frac{1}{4g^2}(\partial_\mu A_\nu - \partial_\nu A_\mu)^2 + i \sum_r A_\tau(r)N(-1)^{x+y+z},$$

(6.3)

where $N$ is the magnitude of the staggered gauge charge for the $U(1)$ gauge field residing
on the two sublattices of the (bipartite) cubic lattice. That is, there exist background
gauge charges $(-1)^{x+y+z}N$ at the lattice points $(x,y,z)$. As will become clear later, these
background charges are the source of the Berry phases experienced by monopoles (or dyons).
The existence of the background charges on the lattice for the monopoles /dyons can be
seen from the following argument. If there were no background charge, the dispersion of
monopoles/dyons on the dual lattice would have the minimum at the zero crystal momentum.
The confinement transition via the condensation of monopoles/dyons would occur at the
zero crystal momentum. This would suggest that the resulting paramagnetic insulator (with
a charge gap) would not break any translational symmetry and at the same time there
would be no ground state degeneracy. When the number of spins in the unit cell is odd,
which is the case of interest here, this is not possible because the translationally invariant
paramagnetic ground states in such cases can only have either a gapped phase with a ground
state degeneracy or a gapless phase via the Hasting’s theorem[165]. Currently there is
no straightforward method to derive the Berry phases or the background gauge charges
starting from the first principles in the fermionic spin liquid cases, while such a procedure
is well understood in bosonic spin liquid phases[166, 167]. In this work, we will work with a
representative background charge distribution with the crustal momentum $q = (\pi, \pi, \pi)$ in
the cubic lattice. Other crystal momentum can arise depending on the lattice structure and
nearby short-range magnetic fluctuations.
The second term $L_\theta$ of Eq. (6.2) is the axion term for the emergent compact $U(1)$ gauge field, arising from the topological properties of the spinons:

$$L_\theta = \frac{\theta}{8\pi^2} \varepsilon^{\mu\nu\lambda\rho} \partial_\mu A_\nu \partial_\lambda A_\rho.$$  (6.4)

To perform a duality transformation on the corresponding action,

$$S_A = \int d\tau d^3r \left( \frac{1}{4g^2} (\partial_\mu A_\nu - \partial_\nu A_\mu)^2 + \frac{\theta}{8\pi^2} \varepsilon^{\mu\nu\lambda\rho} \partial_\mu A_\nu \partial_\lambda A_\rho + i \sum_r A_x(r) N(-1)^{x+y+z}, \right.$$  (6.5)

we introduce the monopole current $m_\mu = \frac{1}{4\pi^2} \varepsilon^{\mu\nu\lambda\rho} \partial_\nu S_\lambda \rho$, where $S_\lambda \rho \in 2\pi \mathbb{Z}$ so that $m_\mu \in \mathbb{Z}$. Introduction of the monopole field $m_\mu$ modifies $S_A$ such that $\partial_\mu A_\nu - \partial_\nu A_\mu \rightarrow \partial_\mu A_\nu - \partial_\nu A_\mu + S_\mu$. Since the action is quadratic in $A_\mu$, we can formally integrate out $A_\mu$. In order to do so, we first solve the Gauss law constraint for the “electric” field of the $U(1)$ gauge theory, namely $\nabla \cdot \vec{E} = N(-1)^{x+y+z}$, by breaking the gauge field $A_\mu$ into the fluctuating part $a_\mu$ (which is free of the constraint) and the static field $a_\mu^0$ that is responsible for the staggered gauge charge. That is, we write $A_\mu = a_\mu + a_\mu^0$ and integrate out $a_\mu$. This generates only two terms that are simple and intuitively understandable:

$$S = \int d\tau d^3r \left( \frac{G^2}{2} m^\mu \frac{1}{\partial^2} m_\mu + i (X_0^\mu + \frac{\theta}{2\pi} a_\mu^0 m_\mu) \right).$$  (6.6)

The first term describes the Coulomb interaction $\sim -\frac{1}{r^2}$ between dyons with the modified strength $G^2 = (\frac{g^2}{2\pi^2})^2 + \frac{4\pi^2}{g^2}$ due to the “electric” charge $g/2 = g \times \frac{\theta}{2\pi}$ with $\theta = \pi$ and “magnetic” charge $2\pi$. The second term represents the Berry phase experienced by the dyons due to the staggered QED charge $\nabla \cdot \vec{E} = N(-1)^{x+y+z}$. Here, $X_0^\mu$ is the dual $U(1)$ gauge field for $a_\mu^0$. This has the form of the minimal couplings of $m_\mu$ to $a_\mu^0$ and $X_0^\mu$, and simply dictates that the monopole carries the $U(1)$ gauge charge $\theta/2\pi$ and the unit magnetic charge $2\pi$ as expected from the axion term.

We now derive the dyon action in Eq. (6.6) rigorously, and also show that there is no long-range statistical interaction between the dyons, that is, that the statistics of the monopoles does not experience any statistical transmutation when they are converted to dyons. We begin with the Lagrangian of the action $S_A$ in Eq. (6.5) with $A_\mu = a_\mu + a_\mu^0$ where $a_\mu^0$ represents the static configuration due to the background gauge charge $N(-1)^{x+y+z}$. Splitting the Lagrangian in terms of $a_\mu^0$ and $a_\mu$, and using $f_{\mu\nu} = \partial_\mu a_\nu - \partial_\nu a_\mu$ and $f_{\mu\nu}^0 = \partial_\mu a_\nu^0 - \partial_\nu a_\mu^0$, the resulting Lagrangian can be written as

$$L = L_1[a_\mu, S_\mu] + L_2[a_\mu^0, S_\mu] + L_3[a_\mu, a_\mu^0].$$  (6.7)
The Lagrangian for the purely fluctuating part, $L_1$, consists of the standard QED$_4$ supplemented by the axion term in the presence of the monopole currents.

$$
L_1[a_\mu, S_{\mu\nu}] = \frac{1}{4g^2} (f_{\mu\nu} + S_{\mu\nu})^2 + \frac{\theta}{16\pi^2} \varepsilon^{\mu\nu\lambda\rho} f_{\mu\nu} S_{\lambda\rho} \\
+ \frac{\theta}{32\pi^2} \varepsilon^{\mu\nu\lambda\rho} S_{\mu\nu} S_{\lambda\rho} + \frac{\theta}{32\pi^2} \varepsilon^{\mu\nu\lambda\rho} f_{\mu\nu} f_{\lambda\rho} 
$$

The other parts of the Lagrangian are given by

$$
L_2[a_0^0, S_{\mu\nu}] = \frac{1}{4g^2} (f_{\mu\nu}^0)^2 + i\eta^\mu a_0^0 \\
+ \frac{1}{2g^2} f_{\mu\nu}^0 S_{\mu\nu} + \frac{\theta}{16\pi^2} \varepsilon^{\mu\nu\lambda\rho} f_{\mu\nu}^0 S_{\lambda\rho},
$$

where $\eta^\mu = N(-1)^{x+y+z}\delta^{\mu,\tau}$ encoding the staggered QED charge, and the mixed contributions

$$
L_3[a_\mu, a_0^0] = \frac{1}{2g^2} f_{\mu\nu}^0 f_{\mu\nu} + \frac{\theta}{16\pi^2} \varepsilon^{\mu\nu\lambda\rho} f_{\mu\nu}^0 S_{\lambda\rho}. 
$$

Up to this point, there have been no approximations. We now transform each term into a desired form via approximations justified in the limit of the large mass gaps for the monopole and the spinon. We begin by dropping $L_3[a_\mu, a_0^0]$ entirely using $\partial_\mu f_{\mu\nu} \sim 0$ and $\varepsilon^{\mu\nu\lambda\rho} \partial_\nu f_{\lambda\rho} = 0$. The first condition $\partial_\mu f_{\mu\nu} \sim 0$ is satisfied if the gap for “charged” excitations is large enough that there is no free current giving rise to a field strength. In the Coulomb phase, every matter field (including monopoles and dyons) is gapped so this approximation is justified.

For $L_2$, we solve $\frac{1}{4g^2} (f_{\mu\nu}^0)^2 + i\eta^\mu a_0^0$ first to fix $a_0^0$ and end up with the following Lagrangian

$$
L_2[a_0^0, S_{\mu\nu}] = \frac{1}{2g^2} f_{\mu\nu}^0 f_{\mu\nu} + \frac{\theta}{16\pi^2} \varepsilon^{\mu\nu\lambda\rho} f_{\mu\nu}^0 S_{\lambda\rho} \\
= X_\mu^0 m_\mu + \frac{\theta}{2\pi} a_\mu^0 m_\mu, 
$$

where the equality $f_{\mu\nu}^0 = \frac{2\pi}{g^2} \varepsilon_{\mu\nu\lambda\rho} \partial_\lambda X_\rho^0$ ($X^0 \sim$ dual $U(1)$ gauge field) and $m_\mu = \frac{1}{4\pi} \varepsilon_{\mu\nu\lambda\rho} \partial_\nu S_{\lambda\rho}$ are used. Thus, $L_2$ contains all the important Berry phase terms for the monopole operator.

Now we integrate out $a_\mu$ in $L_1$ to investigate the Coulomb interaction between monopoles and the statistical interaction. We choose the radiation gauge for the fluctuating $U(1)$ gauge field $a_\mu$ (i.e., we use the “photon” propagator $\frac{g^2}{2\pi}\frac{1}{\partial^2}$) to obtain

$$
L_1 = \frac{1}{2} \left( \frac{g\theta}{2\pi} m_\mu \frac{\partial}{\partial^2} m_\mu + \frac{1}{4g^2} (S_{\mu\nu}^2 + 2\partial_\mu S_{\alpha\mu} \frac{1}{\partial^2} \partial_\nu S_{\alpha\nu}) \\
+ \frac{\theta}{32\pi^2} \varepsilon^{\mu\nu\lambda\rho} S_{\mu\nu} S_{\lambda\rho} + \frac{\theta}{8\pi^2} \partial_\nu S_{\mu\nu} \frac{1}{\partial^2} \varepsilon^{\mu\alpha\beta\rho} \partial_\alpha S_{\beta\rho},
$$

Straightforward calculation reveals that the first line in the above $L_1$ becomes the Coulomb interaction between dyons and the second line exactly vanishes, i.e., $\frac{1}{32\pi^2} \varepsilon^{\mu\nu\lambda\rho} S_{\mu\nu} S_{\lambda\rho} + \frac{\theta}{32\pi^2} \varepsilon^{\mu\nu\lambda\rho} S_{\mu\nu} S_{\lambda\rho}$.
\frac{1}{8\pi}\partial_{\nu}S_{\mu\nu}\frac{1}{2\pi}\varepsilon^{\alpha\beta\rho}\partial_{\alpha}S_{\beta\rho} = 0 \text{ up to the boundary terms. We are discussing the bulk transition without boundary, hence this term can be dropped out completely. In fact, this term corresponds to the } \theta \text{-dependent statistical interaction between the dyons as discussed in A. Goldhaber et.al.} [148, 160] \text{ Hence, the dyons do not receive additional statistical interaction among themselves. This suggests that the dyon in the topological Mott insulator is bosonic and can be condensed. Using } \theta = \pi \text{ and collecting the resulting terms in } L_1 + L_2 + L_3, \text{ we arrive at the effective action for the dyons}

\begin{align*}
S = \int d\tau d^3r \left( \frac{G^2}{2} m^\mu \frac{1}{-\theta^2} m_\mu + i(X_0^\mu + \frac{1}{2} a_0^0 m^\mu) \right),
\end{align*}

(6.13)

as advertised before. To proceed further, we introduce the soft-spin operator \( \psi^\dagger \sim \exp(-i\phi) \) for the dyon creation and put the lattice structure back to obtain the Hamiltonian on the dual lattice.

\begin{align*}
H = -t \sum_{R,R'} \psi^\dagger_R \exp(-i(X_{0R'} + \frac{1}{2} a_0^{0R'} + GL_{RR'})) \psi_{R'} + h.c.,
\end{align*}

(6.14)

where we introduce an auxiliary fluctuating \( U(1) \) gauge field \( L_{RR'} \) to encode the Coulomb interaction with the coupling constant \( G = \sqrt{g^2/4 + 4\pi^2/g^2} \), and \( R \) denotes a dual lattice site.

Some comments on this Hamiltonian are in order. First of all, we need to be careful in defining \( a_0^{0R'} \) on the dual link as \( a_0^0 \) was originally meaningful on the links of the direct lattice. To resolve this issue, we need to introduce a short-ranged function \( F_{RR'}^\lambda \) which maps the direct link to the dual link. This defines \( a_0^{0R'} = \sum_{<rr'>} F_{rr'}^{RR'} a_0^{0r} \). The appearance of this short-ranged function \( F_{rr'}^{RR'} \) can be traced back to the form of the axion term which connects \( f_{\mu\nu} \) to \( f_{\lambda\rho} \) by \( \varepsilon^{\mu\nu\lambda\rho} \) and we are forced to introduce such a function [148, 149] if we wish to study the axion term on the lattice. Secondly, we have introduced an auxiliary non-compact \( U(1) \) gauge field \( L_{RR'} \) which differs from \( a_{RR'} \) and \( X_{RR'} \). In fact, this fluctuating gauge field corresponds to the \( U(1) \) gauge field which is rotated in the electric-magnetic charge. This gauge field is introduced only for convenience as there is no corresponding physical charge. The two physical charges in the dyon theory are the “electric” charge and “magnetic” charge of the compact \( U(1) \) gauge theory \( A_\mu \). However, dyons carry both charges, and the effective Coulomb interaction between the dyons is the sum of the Coulomb interactions of “electric” charges and “magnetic” charges. Because of this, the dyons are seen to interact with the gauge charge \( G = \sqrt{g^2/4 + 4\pi^2/g^2} \). This interaction can be written compactly at the cost of introduction of the auxiliary \( U(1) \) gauge field \( L_{RR'} \). As the low-energy physics is determined by the static component, we can ignore this to study the mean field physics [154]. In the case when \( a_{rr'}^0 = 0 \) can be choosen (no flux threading the direct plaquette), we need to solve the following single-particle hopping problem

\begin{align*}
H = -t \sum_{R,R'} \psi^\dagger_R \exp(-iX_{0R'}^{RR'}) \psi_{R'} + h.c.
\end{align*}

(6.15)
This Hamiltonian leads to a set of degenerate energy minima for $\psi_R$. This degeneracy will be lifted by the non-linear terms mixing these degenerate minima. This is the same procedure as used in studies of monopole condensation and the resulting confinement problem.

There is, however, an important difference from the monopole condensate problem: the number of dyon species. We now argue that it is enough to consider one doublet of dyon operators in the low energy limit. To see this, we first note that the monopole of the strength $2\pi$ can collect the $U(1)$ charge $n + 1/2, n \in \mathbb{Z}$ when the axion angle $\theta = \pi$. Then each dyon will have the self-energy $E \sim (n + 1/2)^2 g^2 + 4\pi^2/g^2$. Thus, the dyon of the monopole strength $2\pi$ has two degenerate states with the charge $1/2$ and $-1/2$, representing the lowest energy dyons. We label $\psi_1$ and $\psi_2$ as the dyons of the magnetic and electric charge content $(2\pi, 1/2)$ and $(2\pi, -1/2)$. These two fields ($\psi_1, \psi_2$) are connected to each other by the time reversal symmetry as the time-reversal operation $T$ will flip only the strength of the magnetic field, i.e., $T[\psi_1] = \psi_2^\dagger$ and $T[\psi_2] = \psi_1^\dagger$ where $\dagger$ operation (particle to anti-particle operation) flips both of the magnetic and electric charge.

The other way to understand the nature of the doublet is to consider the time-reversal symmetry of the spectrum of the dyon fields. We have the time-reversal symmetry before we condense the dyons. As we have a dyon $\psi_1$ of $(2\pi, 1/2)$, we need to have a time-reversal partner of this state, i.e., $(-2\pi, 1/2)$ which is nothing but the state $\psi_2^\dagger$. Hence, we see that when $\psi_1$ (or $\psi_2$) is condensed, we enter a phase where the time-reversal symmetry is broken. We note that even though the above derivation is for the $U(1)$ gauge theory, similar calculation for $\mathbb{Z}_p$ lattice gauge theory should be possible and indeed has been done by J. Cardy et. al.\cite{148,149} without the background charges.

### 6.3 Dyon condensation and resulting broken symmetry phases

In this section, we study the broken symmetry phases that arise when the condensation of dyons occurs in the topological Mott insulator. As the precise ordering depends on the lattice structure, we specifically work on the cubic lattice. To determine the patterns of the symmetry breaking explicitly, we work out the lattice symmetry of the dyon fields and solve the dyon hopping problem. The effect of lattice symmetries (at least translations and rotations) on the monopole operator has been thoroughly studied in the literature and we build on those results\cite{154}. We consider the dyon hopping problem on the dual lattice defined as

$$H = -t \sum_{a=1,2; R, R'} \psi_{a,R}^\dagger \exp(-iX_0^{RR'}) \psi_{a,R'} + h.c,$$ \hfill (6.16)

where we choose $X_0^{RR'}$ that is consistent with the background charge $(-1)^{x+y+z}$. Although here we work on the cubic lattice with the staggered background charge $N = 1$ in Eq.(6.15), it should be straightforward to generalize this for different bipartite lattices and larger $N \in \mathbb{Z}$. For example, a larger staggered charge $N = 2$ on the cubic lattice has been studied for
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the ordinary confined phase, and $N = 2$ background charges were found to induce similar patterns as the case of $N = 1$.[155]

In the case of $N = 1$[154], we have two minima for each $\psi_a$ where the dyon operator takes its minimum kinetic energy. We label these two minima by $\sigma = 1, 2$ and hence we have a total of four operators $\psi_{a,\sigma}, a = 1, 2, \sigma = 1, 2$. The corresponding eigenfunctions[154] have the forms:

$$\psi_{a,1} = \frac{1 + (\sqrt{3} - \sqrt{2})e^{i\pi z}}{\sqrt{2(3 - \sqrt{6})}} e^{i\pi x} - ie^{i\pi y} \sqrt{2} \times \sqrt{2(3 - \sqrt{6})},$$

$$\psi_{a,2} = \frac{1 - (\sqrt{3} - \sqrt{2})e^{i\pi z}}{\sqrt{2(3 - \sqrt{6})}} e^{i\pi y} - ie^{i\pi x} \sqrt{2}.$$ 

Hence, we introduce the dyon operators as follows.

$$\Psi(R, \tau) = \sum_{a,\sigma} \psi_{a,\sigma}(R, \tau)$$  \hspace{1cm} (6.17)

The operations of the spatial symmetries on $\psi_{a,\sigma}$ are worked out in the reference[154], and quoting their results, we get

$$T_x : (\Psi_{a,1}, \Psi_{a,2}) \rightarrow (\Psi_{a,1}^*, -\Psi_{a,2}^*)$$

$$T_y : (\Psi_{a,1}, \Psi_{a,2}) \rightarrow (\Psi_{a,2}^*, \Psi_{a,1}^*)$$

$$T_z : (\Psi_{a,1}, \Psi_{a,2}) \rightarrow (\Psi_{a,2}^*, \Psi_{a,1}^*)$$

$$R_z : (\Psi_{a,1}, \Psi_{a,2}) \rightarrow (e^{i\pi/4} \Psi_{a,1}, e^{i\pi/4} \Psi_{a,2})$$

$$R_y : (\Psi_{a,1}, \Psi_{a,2}) \rightarrow (\frac{\Psi_{a,1}^* + \Psi_{a,2}^*}{\sqrt{2}}, \frac{\Psi_{a,1}^* - \Psi_{a,2}^*}{\sqrt{2}}).$$  \hspace{1cm} (6.18)

Note that the spatial symmetries do not mix the dyons with different $U(1)$ gauge charges, i.e., the translations and rotations do not change the index $a = 1, 2$. To change $a$, we need to consider the time-reversal operation on $\Psi_{a,\sigma}$ because $T[\Psi_{1,\sigma}] = \Psi_{2,\sigma}^*$ and $T[\Psi_{2,\sigma}] = \Psi_{1,\sigma}^*$. The time-reversal operation does not change the index $\sigma$ because (1) the dyon operator in the dual theory does not change the sign (i.e., $T : t_{RR'} \rightarrow t_{RR'}$), and hence no change is involved for the minima of the kinetic energy of the dyon operators (2) the minima of the kinetic energy of the dyon operators are at the time-reversal symmetric momentum. Hence, the spatial symmetry is completely determined by the actions on $\sigma$. We are now ready to introduce the following two vector order parameters

$$\vec{E}_r = \frac{\Psi_{1,\alpha}^* \sigma^{\alpha\beta} \Psi_{1,\beta} + \Psi_{2,\alpha}^* \sigma^{\alpha\beta} \Psi_{2,\beta}^*}{2}$$

$$\vec{B}_r = \frac{\Psi_{1,\alpha}^* \sigma^{\alpha\beta} \Psi_{1,\beta} - \Psi_{2,\alpha}^* \sigma^{\alpha\beta} \Psi_{2,\beta}^*}{2}.$$  \hspace{1cm} (6.19)
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for \( r = x, y, z \). For \( \vec{V} = \vec{E}, \vec{B} \), we have the following transformation rules

\[
\begin{align*}
T_x : (V_x, V_y, V_z) &\rightarrow (-V_x, V_y, V_z) \\
T_y : (V_x, V_y, V_z) &\rightarrow (V_x, -V_y, V_z) \\
T_z : (V_x, V_y, V_z) &\rightarrow (V_x, V_y, -V_z) \\
R_z : (V_x, V_y, V_z) &\rightarrow (V_y, V_x, V_z) \\
R_y : (V_x, V_y, V_z) &\rightarrow (V_z, V_y, V_x)
\end{align*}
\]

(6.20)

The vectors \( \vec{V} = \vec{E}, \vec{B} \) follow the same spatial symmetry transformation rules because the spatial symmetry is fully determined by the actions on \( \sigma \) in \( \Psi_{\alpha, \sigma}, \alpha = 1, 2, \sigma = 1, 2 \). In addition to the lattice symmetry, we also need to introduce the time reversal symmetry operations:

\[
T : (\vec{E}, \vec{B}) = (\vec{E}, -\vec{B}).
\]

(6.21)

In the end, we have two vector operators \( \vec{E} \) and \( \vec{B} \). What phases do these two vector operators \( \vec{E} \) and \( \vec{B} \) represent? It can be shown that the field \( \vec{E} \) behaves like staggered bond order (equivalently, electric flux) and \( \vec{B} \) behaves like staggered current order (magnetic flux).

If the confinement induces ordering of the magnetic degrees of freedom, then the dual operators \( \vec{E} \) and \( \vec{B} \) should have representations in terms of the spin operators \( 154, 155 \). In the previous studies, it is already noticed that \( \vec{E} \) represents the VBS-like order parameters \( 154, 155 \). More explicitly, \( E_x \sim (-1)^x \langle \vec{S}_r \cdot \vec{S}_{r+\hat{x}} \rangle \) and there are analogous identifications for \( E_y \) and \( E_z \). This VBS corresponds to “confined electric flux”.

It is not difficult to see that the magnetic flux expected in the dyon-condensed phase is the field \( \vec{B} \). This magnetic flux should be sourced by the spinon current living on the plane perpendicular to the \( \vec{B} \). In turn, the spinon current can be related to the scalar spin chirality. These facts, hand-in-hand, lead us to the conclusion that the scalar spin chirality can be connected to the vector field \( \vec{B} \). This intuition is supported by explicit construction of appropriate combinations of the scalar spin chirality, which follow the same transformation rules as \( \vec{B} \).

\[
B_x = (-1)^x M_{yz}, B_y = (-1)^y M_{zx}, B_z = (-1)^z M_{xy}
\]

(6.22)

where \( M_{ij} \) is the scalar spin chirality defined on the \( ij \)-plane. For example, \( M_{xy} \) involves four spins of the plaquette on the direct lattice. We label four sites \( 1 = (x, y, z), 2 = (x+1, y, z), 3 = (x+1, y+1, z) \) and \( 4 = (x, y+1, z) \) in the \( xy \)-plane. Then, \( M_{xy} \) is defined uniformly on every plaquette of the \( xy \)-plane as

\[
M_{xy} = \langle \vec{S}_1 \cdot \vec{S}_2 \times \vec{S}_3 \rangle + \langle \vec{S}_2 \cdot \vec{S}_3 \times \vec{S}_4 \rangle + \langle \vec{S}_3 \cdot \vec{S}_4 \times \vec{S}_1 \rangle + \langle \vec{S}_4 \cdot \vec{S}_1 \times \vec{S}_2 \rangle.
\]

(6.23)

It can be shown that \( (-1)^z M_{xy} \) and \( B_z \) follow the same transformation rules under the lattice symmetries and time-reversal symmetry operations. Analogous expressions hold for \( B_y \) and \( B_z \) (as noted before, the scalar spin chirality lies in the plane perpendicular to the vector \( \vec{B} \)).
Thus, we confirm that the scalar spin chirality is induced in the dyon condensed phase. Now we discuss where the scalar spin chirality order comes from. The current order $\vec{B}$ originates from the ‘mixing’ of the two dyon species with different $U(1)$ gauge charges. This order parameter would have not been present if there were only one monopole species as in the usual confinement problem. In the case of the dyon condensate, both of the electric flux and magnetic flux should be confined at the same time. This implies that there should be sources of the magnetic flux as well as the electric flux. We can easily anticipate that the magnetic flux ($\sim \vec{B}$) can arise from the spinon current ($\sim M_{ij}$) via the elementary Biot-Savart Law.

With these identifications between the dyon operators and the corresponding order parameters, we can now ask what kind of phases will eventually appear. This requires the studies of the quartic order and higher order terms in the Landau-Ginzburg theory\cite{154,155} written in terms of the dyon fields $\vec{\Psi}_a^T = (\Psi_{a,1}, \Psi_{a,2}), a = 1, 2$. We will not attempt to solve the full phase diagram but will point out a few representative confined phases from the symmetry-allowed forms of the Landau-Ginzburg theory

$$L = L_{\text{kin}}(\vec{\Psi}_1) + L_{\text{kin}}(\vec{\Psi}_2) + L_{\text{int}}(\vec{\Psi}_1, \vec{\Psi}_2).$$

(6.24)

Here, $L_{\text{kin}}$ represents the kinetic terms in Eq.(6.15). We expand $L_{\text{int}} = L_2 + L_4 + \cdots$ with $L_n \sim O(\vec{\Psi}^n)$, $n \in \mathbb{Z}$. By requiring the lattice symmetry and the time-reversal symmetry, we identify $L_2 = r|\vec{\Psi}_1|^2 + r|\vec{\Psi}_2|^2$ and

$$L_4 = u(|\vec{\Psi}_1| \cdot \vec{\Psi}_1|^2 + u(|\vec{\Psi}_2|^2 v|\vec{\Psi}_1|^2 + w|\vec{\Psi}_1 \cdot \vec{\Psi}_2|^2.$$  

(6.25)

Up to this quartic order, we notice that there are several interesting possibilities. First, $\langle \vec{\Psi}_1 \rangle = 0$ and $\langle \vec{\Psi}_2 \rangle = 0$ for $r > 0$: This phase is the topological Mott insulator phase. The order parameters are $\vec{E} = 0$ and $\vec{B} = 0$. Secondly, when the sign of the mass term for $\vec{\Psi}_a$ is negative $r < 0$ in $L_2$, two dyon fields $\vec{\Psi}_1$ and $\vec{\Psi}_2$ tend to condense. We assume $u > 0$ in $L_4$. There are four following possibilities of $L_4$.

(1) If $w < 0$ and $2u > v > -2u$, we have $\langle \vec{\Psi}_1 \rangle = \vec{\rho} \exp(i\phi_1), \langle \vec{\Psi}_2 \rangle = \vec{\rho} \exp(i\phi_2)$ where $\vec{\rho}$ is a real two-component spinor. Then, the order parameter $\vec{E} \propto \vec{\rho}^T \sigma \vec{\rho} \neq 0$ but $\vec{B} = 0$. The two dyon fields condense at the equal amplitude in a way to respect the time-reversal symmetry. Hence $\vec{B} = 0$ is inevitable, and this phase is the ordinary confined phase.

(2) If $w > 0$ and $v > 2u$, then we have $\langle \vec{\Psi}_1 \rangle \neq 0$ but $\langle \vec{\Psi}_2 \rangle = 0$. Here, $\vec{E}$ and $\vec{B}$ acquire non-zero expectation values (with $\vec{E} \parallel \vec{B}$) at the same time, and in this phase, the scalar spin chirality and the VBS order coexist. Furthermore, the time-reversal symmetry is spontaneously broken.

(3) If $w > 0$ and $2u > v + w > -2u$, we have $\langle \vec{\Psi}_1 \rangle = \vec{\rho}_1 \exp(i\phi_1), \langle \vec{\Psi}_2 \rangle = \vec{\rho}_2 \exp(i\phi_2)$ where $\rho_1$ and $\rho_2$ are the real two-component spinors with $\vec{\rho}_1 \cdot \vec{\rho}_2 = 0$. In this confined phase, the order parameters $\vec{E} = 0$ but $\vec{B} \neq 0$. Thus, this phase corresponds to the phase where only
the scalar spin chirality orders. Here, the two dyon fields condense at the equal amplitude in a way to break the time-reversal symmetry maximally. This phase should be considered as an “opposite” of the phase (1) where only $\vec{E}$ acquires non-zero expectation value.

(4) If $w < 0$ and $v + w > 2u$, the only one of the two dyon fields condenses. The phase is identical to the phase (2) and there are two orders present in the phase.

The detailed spatial patterns of the order parameters can depend on the higher-order terms in $L_{\text{int}}$ which we do not consider (in fact, the pattern depends on the $\sim O(\chi^8)$ in the Landau-Ginzburg theory, see for example Motrunich et.al [154]).

6.4 Conclusion and outlook

In this paper, we have studied the condensation of dyons and the corresponding confined phases in topological Mott insulators. Using the effective field theory and projective symmetry analysis on the dyon operators, we identified possible broken symmetry phases resulting from such confinement. Because the dyons are monopoles endowed with gauge charge, the confined phase can induce at least two different orders: bond order and current order. In the case when the axion angle $\theta$ is not $\pi$, we might need to consider more species of the dyons. However, the dyon carries the “electric” and “magnetic” charges as far as $\theta \neq 0$, and this implies that the confined phase in the non-zero axion angle $\theta$ will be a coexisting phase of the bond order and the current order if $\theta \neq 0$.

For the physical spin/magnetic degree of freedom, the physical order parameters in the confined phase were shown to be the scalar spin chirality order and the VBS order. It should be emphasized that the coexistence of two order parameters discussed above is unique to the confined phase of the topological Mott insulators and does not arise in ordinary confinement physics in condensed matter systems. Thus the emergence of the coexisting scalar spin chirality and VBS orders via a second order transition from a quantum paramagnet would be strong evidence that such a quantum paramagnet was in fact the topological Mott insulator.

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Chapter 7

Two dimensional symmetry protected topological phases with PSU(N) and time reversal symmetry

The interplay between strong interaction and strong quantum fluctuation can lead to many remarkable properties in quantum disordered phases. In the most trivial case, a quantum disordered phase is fully gapped, and nondegenerate, and its ground state wave function can be adiabatically connected to a direct product wave function without any phase transition. These quantum disordered phases are “trivial”, in the sense that they are quantum analogues of classical disordered phases, i.e. they are completely featureless. The best example of trivial quantum disordered phase is the Mott insulator phase of spinless bosonic atoms trapped in an optical lattice. Every state of this Mott insulator can be adiabatically connected to direct product state \( \prod_i | \hat{n}_i = k \rangle_i \), where \( \hat{n}_i \) is the boson number operator on site \( i \), and \( k \) is an integer.

The description of trivial quantum disordered phases is semiclassical, i.e. we can describe the trivial quantum disordered phase using a semiclassical field theory defined with a Landau order parameter. For example, a trivial quantum disordered phase of a system with SO(3) spin rotation symmetry can be described by a semiclassical nonlinear sigma model (NLSM) defined with the semiclassical Néel order vector \( \vec{n} \) with unit length \( (\vec{n})^2 = 1 \):

\[
S = \int d^d x d\tau \frac{1}{g} (\partial_{\mu} \vec{n})^2.
\]  

(7.1)

In spatial dimensions higher than 1, by tuning the parameter \( g \), there is an order-disordered phase transition: when \( g < g_c \), \( \vec{n} \) is ordered, and the SO(3) symmetry is spontaneously broken; when \( g > g_c \), \( \vec{n} \) is disordered, and the ground state wave function of this quantum disordered phase is approximately a direct product state \( |0\rangle \sim \prod_i |l = 0\rangle_i \), where \( l \) is the angular momentum quantum number on every site.

Now there is a consensus that, quantum disordered phases of strongly correlated systems can have much richer structures compared with classical disordered phases. So far there are
three types of “nontrivial” quantum disordered phases: (i.) topological phases, whose ground state is fully gapped but topologically degenerate; (ii.) Algebraic spin (Bose) liquid phase, which is still a quantum disordered phase of a bosonic spin system, but the spectrum remains gapless, and the physical quantities have a power-law instead of short range correlation; (iii.) Symmetry protected topological (SPT) phases, whose bulk spectrum is identical to a trivial quantum disordered phase, but its boundary must be either gapless or degenerate when and only when the system has certain symmetry $G$. The ground state wavefunction of a SPT is completely different and cannot be continuously connected to a trivial wave function without a phase transition, when the Hamiltonian is invariant under symmetry $G$. The 2d quantum spin Hall insulator and the 3d topological insulator are both SPT phases with time-reversal symmetry.

In this work we will focus on SPT phases of bosonic spin systems. SPT is a pure quantum phenomenon, and there is no analogue in classical world. Thus one would expect that the description for these states should be purely quantum, and a semiclassical formalism should completely fail to describe them. However, we will try to demonstrate that, the SPT phases can still be described semiclassically using NLSMs like Eq. 7.1 as long as there is an appropriate topological term. We want to stress that, in our approach, the target space of the NLSM is the manifold of a semiclassical order parameter. This is different from the NLSMs discussed in Ref. [18, 22], where a NLSM was also introduced to describe SPT, but the target space of this NLSM is the group manifold of the symmetry $G$, instead of a semiclassical order parameter.

At least in one dimensional systems, semiclassical NLSMs have been proved successful in describing SPT phases. For example, the O(3) NLSM in Eq. 7.1, plus a topological $\Theta$–term describes a spin-1 Heisenberg chain when $\Theta = 2\pi$, and it is well-known that the spin-1 antiferromagnetic Heisenberg model is a SPT phase with 2-fold degeneracy at each boundary [168, 169]. This two fold degeneracy at the boundary can be read off from this 1d O(3) NLSM, since its boundary is a 0+1d O(3) NLSM with a Wess-Zumino-Witten term at level $k = 1$, whose ground state is two fold degenerate [170].

In Ref. [171], the author discussed a class of three dimensional SPT with SU($N$) symmetry (Rigorously speaking, the symmetry of the SPT constructed in Ref. [171] is PSU($N$) = SU($N$)/$Z_N$, where $Z_N$ is the center of SU($N$)), and just like the Haldane phase in 1d, this 3d SPT is described by a NLSM defined with the Néel order parameter only. For SU($N$) magnet, the manifold $\mathcal{M}$ of the Néel order is $\mathcal{M} = \frac{U(N)}{U(m) \times U(N-m)}$ [172, 173]. When $N > 2$ and $1 < m < N - 1$, $\pi_4[\mathcal{M}] = Z$. Thus a nontrivial topological $\Theta$–term can be defined for the SU($N$) Néel order parameter, and when $\Theta = 2\pi$, it was argued that the system is a three dimensional SPT, whose 2+1d boundary must be either gapless or degenerate [171].

In 2 dimensional space, a straightforward generalization of Ref. [171] is difficult, since for $N > 2$, $\pi_3[\frac{U(N)}{U(m) \times U(N-m)}] = Z_4$, thus a $\Theta$–term is not well defined for manifold $\mathcal{M}$ in two dimensions with general $N$. For the simplest case with $N = 2$ and $m = 1$, i.e. the ordinary SU(2) Néel order whose manifold is $S^2$, although the homotopy group $\pi_3[S^2] = Z$, a nontrivial mapping from the space-time manifold to the target space $S^2$ cannot be written as an integral
of local terms of the Néel order parameter, thus it is much more complicated. Alternatively, in this paper we will study 2d systems with symmetry \( \text{PSU}(N) \times \mathbb{Z}_2^T \), where \( \mathbb{Z}_2^T \) is the time-reversal symmetry. We will demonstrate that for a system with \( \text{PSU}(N) \times \mathbb{Z}_2^T \) symmetry, a topological \( \Theta \)-term can be defined in 2+1 dimensional space-time with semiclassical order parameters, and when \( \Theta = 2\pi \) the topological term will drive the system into a SPT phase.

### 7.1 Field theory description

#### 7.1.1 SPT phase at \( \Theta = 2\pi \)

In this section we will discuss the field theory description of the 2+1d SPT with \( \text{PSU}(N) \times \mathbb{Z}_2^T \) symmetry. As we discussed in the introduction, we will take the semiclassical formalism, and define the field theory in terms of the order parameter of \( \text{PSU}(N) \), whose configurations form manifold \( \mathcal{M} = \left( \frac{U(N)}{U(m) \times U(N-m)} \right) \). Every element \( \mathcal{P} \) of the manifold \( \mathcal{M} \) can be represented as

\[
\mathcal{P} = V^\dagger \Omega, \quad \Omega = \begin{pmatrix} 1_{m \times m}, & 0_{m \times N-m} \\ 0_{N-m \times m}, & -1_{N-m \times N-m} \end{pmatrix}, \tag{7.2}
\]

where \( V \) is a \( \text{SU}(N) \) transformation matrix. \( \mathcal{P} \) is a Hermitian matrix, and it is an analogue of the ordinary Néel vector. In fact, when \( N = 2 \), \( \mathcal{M} \) is precisely \( S^2 \). Matrix order parameter \( \mathcal{P} \) is always invariant under the center \( Z_N \) of \( \text{SU}(N) \): \( V = e^{i2\pi/N}1_{N \times N} \), thus a NLSM defined with \( \mathcal{P} \) has symmetry \( \text{PSU}(N) = \text{SU}(N)/Z_N \). When \( N = 2 \), \( \text{PSU}(2) = \text{SO}(3) \) is the ordinary spin rotation group of model Eq. 7.1. If the symmetry of a quantum spin system is \( \text{SO}(3) \) instead of \( \text{SU}(2) \), then the Hilbert space on every site of the system must be a representation of \( \text{SO}(3) \), thus we are restricted to integer spin systems only. With integer spins, \( (\mathbb{Z}_2^T)^2 = +1 \).

For a general \( N \), The homotopy group \( \pi_3[\mathcal{M}] = \mathbb{Z}_1 \), thus a NLSM defined with \( \mathcal{P} \) does not have a nontrivial topological \( \Theta \)-term in 2+1d space-time. Thus for a 2+1d system with \( \text{PSU}(N) \) symmetry only, there is no nontrivial SPT that can be described using semiclassical order parameter \( \mathcal{P} \). Now let us combine \( \text{PSU}(N) \) and time-reversal symmetry together, and define the following order parameter \( U \):

\[
U = \cos(\theta)1_{N \times N} + i \sin(\theta)\mathcal{P}. \tag{7.3}
\]

Now \( U \) is a unitary matrix, and \( U \in \text{SU}(N) \). Since \( \pi_3[\text{SU}(N)] = \mathbb{Z} \), a principal chiral nonlinear sigma model can be defined with order parameter \( U \), plus a nontrivial topological \( \Theta \)-term:

\[
S = \int d^2xd\tau \frac{1}{g} \text{tr}[\partial_\mu U^\dagger \partial_\mu U] + \frac{i\Theta}{24\pi^2} \text{tr}[U^\dagger \partial_\mu UU^\dagger \partial_\nu UU^\dagger \partial_\rho U] \epsilon_{\mu\nu\rho}. \tag{7.4}
\]
In the simplest case with \( N = 2 \) and \( m = 1 \), the order parameter \( \mathcal{P} \) is equivalent to an \( O(3) \) vector \( \vec{n} \): \( \mathcal{P} = \vec{n} \cdot \vec{\sigma} \). Then Eq. [7.4] is just an \( O(4) \) NLSM:

\[
\mathcal{S} = \int d^2x d\tau \frac{1}{g} (\partial_\mu \vec{\phi})^2 + \frac{i\Theta}{12\pi^2} \epsilon_{abcd} \epsilon_{\mu\nu\rho} \phi^a \partial_\mu \phi^b \partial_\nu \phi^c \partial_\rho \phi^d,
\]

(7.5)

where \( \vec{\phi} = (\cos(\theta), \sin(\theta)\vec{n}) \).

For general \( N \), the SU(\( N \)) matrix \( U \) has a SU(\( N \))\_\text{left} transformation and a SU(\( N \))\_\text{right} transformation, but there are higher order terms in the Eq. [7.4] that break the two SU(\( N \)) symmetries down to its diagonal subgroup PSU(\( N \)). Under symmetry PSU(\( N \)) \( \times \mathbb{Z}_2^T \), the order parameters transform as

\[
\begin{align*}
\text{SU}(\! N \!) & : \ U \rightarrow V^\dagger UV, \\
\mathbb{Z}_2^T & : \mathcal{P} \rightarrow \mathcal{P}^*, \quad \theta \rightarrow \pi - \theta, \quad U \rightarrow -U^t.
\end{align*}
\]

(7.6)

In the follows, we will argue that, when \( \Theta = 2\pi \), Eq. [7.4] with symmetry SU(\( N \)) \( \times \mathbb{Z}_2^T \) describes a SPT, whose 1+1d boundary must be either gapless or degenerate.

In Eq. [7.4] by tuning \( g \), there is an order-disorder phase transition. We will always focus on the disordered phase of Eq. [7.4] thus we will focus on the phase with a large coupling constant \( g \). When \( \Theta = 2\pi \), the bulk spectrum of the quantum disordered phase is identical to the case with \( \Theta = 0 \), thus the bulk is fully gapped and nondegenerate. Then one can safely integrate out the bulk and focus on the boundary. At \( \Theta = 2\pi \), the edge is described by the following principal chiral model with a Wess-Zumino-Witten (WZW) term:

\[
\mathcal{S}_b = \int dx d\tau \frac{1}{g} \text{tr}[\partial_\mu U^\dagger \partial_\mu U] + \int dx d\tau du \frac{i\Theta}{24\pi^2} \text{tr}[U^\dagger \partial_\mu U U^\dagger \partial_\nu U U^\dagger \partial_\rho U] \epsilon_{\mu\nu\rho}.
\]

(7.7)

Here \( U(x, \tau, u) \) is an extension of physical order parameter \( U(x, \tau) \) that satisfies

\[
\begin{align*}
U(x, \tau, u = 0) &= 1_{N \times N}, \\
U(x, \tau, u = 1) &= U(x, \tau).
\end{align*}
\]

(7.8)

For the simple case with \( N = 2m = 2 \), Eq. [7.7] reduces to a 1+1d O(4) NLSM with a WZW term at level-1:

\[
\mathcal{S} = \int dx d\tau \frac{1}{g} (\partial_\mu \vec{\phi})^2
\]
This principal chiral model Eq. (7.7), with a full SU($N_{\text{left}} \times SU(N_{\text{right}})$) symmetry, is proved to be gapless, and it is described by the SU($N$)$_1$ conformal field theory\cite{174,175}. However, in our system the SU($N_{\text{left}} \times SU(N_{\text{right}})$) symmetry is broken down to the diagonal SU($N$), thus the conformal field theory might be gapped out due to relevant perturbations introduced by this symmetry reduction. With this symmetry reduction, the boundary theory Eq. (7.7) is reduced to the following NLSM with a $\Theta'$-term:

$$L_b = \frac{1}{g} \text{tr}[(\partial_\mu \mathcal{P})^2] + \frac{\Theta'}{16\pi} \text{tr}[\mathcal{P} \partial_\mu \mathcal{P} \partial_\nu \mathcal{P}] \epsilon_{\mu\nu},$$

(7.10)

as long as the $Z_2^T$ symmetry is preserved, namely the expectation value of $\cos(\theta)$ is zero, the boundary $\Theta'$ is fixed at $\Theta' = \pi$. Under the $Z_2^T$ transformation, $\Theta' \to 2\pi - \Theta'$. If the time-reversal symmetry is explicitly broken, namely a background field that couples linearly to $\cos(\theta)$ is turned on, then at the boundary $\Theta'$ is also tuned away from $\pi$: $\Theta' = 2\theta - 2\cos(\theta)\sin(\theta)$.

If we ignore the physical interpretation of the field $\mathcal{P}$, this 1+1d NLSM at $\Theta' = \pi$ (Eq. (7.10)) can be used to describe the SU($N$) antiferromagnet with conjugate representations on A and B sublattices\cite{172,173,176}, and $\mathcal{P}$ is precisely the SU($N$) Néel order parameter. In fact, for the simplest case with $N = 2$, $m = 1$, Eq. (7.10) precisely reduces to an O(3) NLSM with a $\Theta'$ term with $\Theta' = \pi$:

$$S = \int dxd\tau \frac{1}{g} (\partial_\mu \vec{n})^2 + \frac{i\Theta'}{8\pi} \epsilon_{abc} \epsilon_{\mu\nu} n^a \partial_\mu n^b \partial_\nu n^c.$$  

(7.11)

With $\Theta' = \pi$, this model describes an antiferromagnetic spin-1/2 chain, and based on the Lieb-Schultz-Mattis (LSM) theorem this theory must be either gapless or degenerate\cite{177}.

In Eq. (7.10), $\Theta' = \pi$ can be viewed as the transition point between two stable fixed points at $\Theta' = 0$ and $2\pi$, and this transition is driven by tuning $\Theta'$. This transition can be analyzed through a renormalization group calculation of both $g$ and $\Theta'$ as in Ref.\cite{178,182}. If this transition is continuous, then this boundary system must be a gapless CFT at $\Theta' = \pi$; if this transition is first order, then this boundary system must be two fold degenerate at $\Theta' = \pi$\cite{183}. Thus we conclude when the bulk theory Eq. (7.4) has $\Theta = 2\pi$, its boundary must be nontrivial, i.e. it must be either gapless or degenerate.

To demonstrate that this phase is a SPT, we need to show that its boundary can only be realized as the boundary of a 2+1d system, i.e. it cannot be realized as a real one dimensional lattice quantum spin system with the same symmetry. For example, the boundary of a 2d quantum spin Hall insulator is a 1d helical Luttinger liquid with central charge 1, and it can be argued that this 1d helical Luttinger liquid cannot be realized as a 1d electron system with time-reversal symmetry\cite{184}. Also, the boundary of 3d topological insulator is a single 2d Dirac cone, which cannot be realized in a pure 2d system with time-reversal symmetry. Let us take the simplest case with $N = 2m = 2$ as an example. In order to argue that Eq. (7.11)
cannot be realized in a 1d system with \( \text{SO}(3) \times \mathbb{Z}_T^T \) symmetry, let us break the time-reversal symmetry at the boundary, but make a domain wall of the time-reversal symmetry breaking pattern:

\[
\Theta' > \pi, \text{ for } x > 0; \quad \Theta' < \pi, \text{ for } x < 0. \tag{7.12}
\]

The two sides of the domain wall are conjugate to each other under time-reversal transformation. Based on the renormalization group calculation of Ref.\[178\text{--}182\], and the argument in Ref.\[183\], when \( \Theta' > \pi \) the system is in the same phase as \( \Theta' = 2\pi \), while when \( \Theta' < \pi \) the system is in the same phase as \( \Theta' = 0 \), both phases are fully gapped and nondegenerate. At the domain wall this system is described by a 0+1d O(3) NLSM with a WZW term at level-1:

\[
S = \int d\tau \frac{1}{g} (\partial_\mu \vec{n})^2 + \int d\tau du \frac{2\pi i}{8\pi} \epsilon_{\mu \nu} \epsilon_{abc} \partial_\mu n^a \partial_\nu n^b \partial_\nu n^c, \tag{7.13}
\]

which is precisely the model describing a single spin-1/2. A spin-1/2 excitation is not a representation of \( \text{SO}(3) \) (it is a representation of \( \text{SU}(2) \)), since it is not invariant under the center of \( \text{SU}(2) \). Also, under the square of time-reversal transformation, the wave function of a spin-1/2 excitation would change sign: \( (\mathbb{Z}_T^T)^2 = -1 \). This implies that physical symmetries fractionalize at the domain wall.

Although one dimensional spin chains can have fractionalized excitations, this phenomenon of deconfined domain-wall fractionalization cannot happen in a one dimensional integer spin chain. Consider for example two 1d systems with integer spins and \( \text{SO}(3) \) symmetry, then if these two systems are conjugate to each other under time-reversal symmetry, then they must be either both 1d SPT, or both trivial states. Then at their domain wall there should be either an integer localized domain wall spin, or no domain wall spin at all.

The analysis of domain wall state at the boundary can be generalized to arbitrary \( N \). Based on all the analysis above, we can conclude that Eq.\[7.4\] with \( \Theta = 2\pi \) is a SPT with symmetry \( \text{PSU}(N) \times \mathbb{Z}_T^T \).

Now let us couple two copies of Eq.\[7.4\] (defined with \( \text{SU}(N) \) matrices \( U_1 \) and \( U_2 \) respectively) together, both theories have \( \Theta = 2\pi \) in the decoupled limit. \( U_1 \) and \( U_2 \) transform identically under \( \text{PSU}(N) \times \mathbb{Z}_T^T \). Then the following couplings are allowed by the symmetry:

\[
\mathcal{L}_c = -A \text{tr}[U_1 U_2] - B \text{tr}[U_1^T U_2] + H.c. \tag{7.14}
\]

In the limit \( A = 0, B = \infty \), \( U_2 \) is effectively equivalent to \( U_1 \), thus the coupled theory is just one copy of \( \text{SU}(N) \) principal chiral model with \( \Theta = 4\pi \); in the other limit \( A = \infty, B = 0 \), \( U_2 \) is effectively \( U_1^T \), and the final theory is effectively one copy of \( \text{SU}(N) \) PCM with \( \Theta = 0 \). By tuning \( A \) and \( B \), these two limits can be connected continuously without any bulk phase transition in between. During this process, however, the effective boundary theory Eq.\[7.10\] evolves from \( \Theta' = 2\pi \) to \( \Theta' = 0 \), thus there must be a boundary transition \( \Theta' = \pi \) between the two limits. Thus \( \Theta = 4\pi \) and \( \Theta = 0 \) are separated by a boundary transition but no bulk transition, \( i.e. \) they are topologically equivalent in the bulk. Based on this observation we
conclude that there are only two classes of 2+1d SPTs with \( \text{PSU}(N) \times \mathbb{Z}_T^2 \) symmetry: there is a trivial class at \( \Theta = 4k\pi \), and nontrivial class at \( \Theta = (4k + 2)\pi \). In Ref.\[18\], using group cohomology, it was concluded that the 2 dimensional SPT phase with \( \text{SO}(3) \times \mathbb{Z}_T^2 \) symmetry has a \( \mathbb{Z}_2 \) classification, which is consistent with our result for general \( N \).

### 7.1.2 Physics with \( \Theta = \pi \)

In Ref.\[183\], it was argued that the quantum disordered phase of the principal chiral model Eq.\[7.4\] must be either gapless or two fold degenerate when \( \Theta = \pi \). In Ref.\[183\] it was assumed that the system has a full \( \text{SU}(N)_{\text{left}} \times \text{SU}(N)_{\text{right}} \) symmetry. In our current case, the actual symmetry is \( \text{PSU}(N) \times \mathbb{Z}_T^2 \). Using a different argument from Ref.\[183\], we will make the same conclusion for Eq.\[7.4\], i.e. its quantum disordered phase cannot be gapped without degeneracy when \( \Theta = \pi \).

In order to argue that a system is either gapless or degenerate when \( \Theta = \pi \), we only need to argue that if the system is gapped, it must be degenerate. Thus let us assume it is gapped in the disordered phase of \( \Theta = \pi \). Under this assumption, the coupling constant \( g \) must flow to infinity in the infrared limit under renormalization group, this is because if \( g \) flows to any fixed point with finite constant \( g^* \), then the system must be scaling invariant and gapless. Thus \( g \) must flow to infinity once we assume the system is gapped. Now let us take \( g \) to infinity, then the first term of Eq.\[7.4\] vanishes, and Eq.\[7.4\] reduces to a pure topological \( \Theta \)-term:

\[
S = \frac{i\Theta}{24\pi^2} \text{tr}[U_+^\dagger \partial_\mu U U_+^\dagger \partial_\nu U_+^\dagger \partial_\rho U] \epsilon_{\mu\nu\rho}. \quad (7.15)
\]

This \( \Theta \)-term contributes phase factor \( \exp(i\Theta) \) to every \( \text{SU}(N) \) instanton in the space-time. However, since our system only has \( \text{PSU}(N) \times \mathbb{Z}_T^2 \) symmetry instead of a full \( \text{SU}(N) \times \text{SU}(N) \) symmetry, an instanton will fractionalize into two monopoles. A monopole centered at the origin has the following configuration:

\[
U = \cos(\theta)1_{N \times N} + i \sin(\theta) \mathcal{P},
\]

\[
\theta(|R| = 0) = 0, \quad \text{or} \quad \pi, \quad \theta(|R| = \infty) = \pi/2;
\]

\[
\int_{|R| = R} d^2R \frac{i}{16\pi} \text{tr}[\mathcal{P} \partial_\mu \mathcal{P} \partial_\nu \mathcal{P}] \epsilon_{\mu\nu} = 1. \quad (7.16)
\]

Here \( \tilde{R} \) is the coordinate in the 2+1d Euclidean space-time. In the simplest case with \( N = 2m = 2 \), this monopole is the ordinary “hedgehog” monopole of vector \( \vec{n} \) in the space-time. When \( \theta = 0 \) and \( \pi \) at the origin \( |\tilde{R}| = 0 \), this monopole carries instanton number 1/2 and \(-1/2\) respectively, thus this monopole contributes phase factor \( \exp(\pm i\Theta/2) \) to the partition function.
Since we are interested in the bulk physics, we can compactify the two dimensional space into a sphere $S^2$. Now let us define the following quantity $\Phi(\tau)$ for every time slice $\tau$:

$$\Phi(\tau) = \int d^2x \frac{i}{32\pi} \text{tr}[\mathcal{P}\partial_i\mathcal{P}\partial_j\mathcal{P}]\epsilon_{ij},$$

and since $\pi_2[\mathcal{M}] = \mathbb{Z}$, $\Phi(\tau)$ is quantized as integer or half-integer, as long as the configuration of $\mathcal{P}$ has no singularity at time $\tau$. $\Phi(\tau)$ is increased and decreased through the monopoles described in the previous paragraph, and one monopole in the space-time changes $\Phi$ by $1/2$:

$$\Phi(\tau = +\infty) - \Phi(\tau = -\infty) = n_m/2.$$

Now under the assumption that the system is gapped (hence $g$ flows to infinity), Eq. 7.4 and Eq. 7.15 reduce to the following single particle quantum mechanics problem defined on a periodic lattice with lattice constant $1/2$:

$$S = \int d\tau \left[ \frac{1}{2}m(\partial_\tau \Phi)^2 \pm i\Theta \partial_\tau \Phi + V(\Phi) \right], \quad m \to 0,$$

where $V(\Phi)$ is a deep periodic potential that makes $\Phi$ takes only integer and half-integer values, thus the original principal chiral model reduces to a single particle tight binding model, where each lattice site corresponds to a quantized value of $\Phi$. Hopping from site $q$ to site $q + 1/2$ corresponds to a monopole in the space-time, and there are two different types of monopole, depending on the sign of $\cos(\theta)$ at the monopole core. The $\Theta$-term will contribute a factor $\exp(i\Theta/2)$ and $\exp(-i\Theta/2)$ to the monopole with $\cos(\theta) = +1$ and $\cos(\theta) = -1$ at the core respectively. With time-reversal symmetry, the two types of monopoles are degenerate, thus when $\Theta = \pi$ these two types of monopoles have complete destructive interference with each other, i.e. hopping by one lattice constant is forbidden. However, hopping by two lattice constants is still allowed, but the band structure will be doubly degenerate, namely on this one dimensional lattice the states with lattice momentum $p = 0$ and $p = 2\pi$ are degenerate.

If $\Theta$ is tuned away from $\pi$, then the nearest neighbor hopping in the tight-binding model Eq. 7.18 is allowed, and the ground state of Eq. 7.18 is nondegenerate. Now we have argued that once the system is gapped at $\Theta = \pi$, it must be two fold degenerate, namely the system must be either gapless or degenerate at $\Theta = \pi$. The analysis in this section implies that when we tune $\Theta = 2\pi$ to $0$, the bulk spectrum must change at $\Theta = \pi$, i.e. the SPT phase and trivial phase must be separated by a bulk transition at $\Theta = \pi$.

### 7.2 Lattice construction for $N = 2$, $m = 1$

In this section we will try to construct a lattice spin state for the 2d SPT with $\text{SO}(3) \times \mathbb{Z}_T^2$ symmetry. Since the Hilbert space on every site must be a representation of $\text{SO}(3)$ group, we must start with an integer spin system. Let us consider a spin-1 system on a honeycomb lattice, and we will construct a spin many-body wave function using the following two-color
Section 7.2. Lattice construction for N = 2, m = 1

slave fermion formalism, which was introduced to understand the spin liquid phenomena observed in Ba$_3$NiSb$_2$O$_9$[180]:

\[ \hat{S}_i^\mu = \frac{1}{2} \sum_{\alpha,\beta=\uparrow,\downarrow} \sum_{a=1,2} f_{\alpha,a,i}^\dagger \sigma_{\alpha\beta}^\mu f_{\beta,a,i}. \] (7.19)

Here \( \sigma^\mu \) are three spin-1/2 Pauli matrices. Each spinon \( f_{\alpha,a} \) has two indices: \( \alpha = \uparrow, \downarrow \) denotes spin and \( a = 1, 2 \) is a “color” quantum number. Thus we can consider not only the usual spin SU(2) rotations in the \( \alpha - \beta \) space, but also color SU(2) transformations in the \( a - b \) space. Matching with the spin Hilbert space requires not only constraining the total fermion number to half-filling (two fermions per site), but also requiring each site to be an color SU(2) singlet, which guarantees that on each site the spin space is a symmetric spin-1 representation:

\[ \hat{n}_i = \sum_{a=1,2} \sum_{\alpha=\uparrow,\downarrow} f_{\alpha,a,i}^\dagger f_{\alpha,a,i} = 2, \]

\[ \hat{\tau}^\mu = \sum_{\alpha,a,b} f_{\alpha,a,i}^\dagger \tau_{ab}^\mu f_{\alpha,b,i} = 0. \] (7.20)

Here \( \tau_{ab}^\mu \) are three Pauli matrices that operate on the color indices. Under time-reversal transformation, in order to satisfy the commutation relation between Pauli matrices, \( \tau^\mu \) should transform just like spin operators: \( \tau^\mu \to -\tau^\mu. \)

Due to these two independent constraints in Eq. (7.20), the spinon \( f_{\alpha,a} \) will have a gauge symmetry. In order to identify the full gauge symmetry, we need to rewrite \( f_{\alpha,a,i} \) in terms of Majorana fermions \( \eta \) as follows:

\[ f_{\alpha,a,i} = \frac{1}{2} (\eta_{\alpha,a,1,i} + i \eta_{\alpha,a,2,i}). \] (7.21)

On every site, \( \eta_i \) has in total three two-component spaces, making the maximal possible transformation on \( \eta_i \) SO(8). Within this SO(8), the spin SU(2) transformations are generated by the three operators

\[ \vec{S} = (\sigma^x \lambda^y, \sigma^y, \sigma^z \lambda^y), \] (7.22)

where the Pauli matrices \( \lambda^a \) operate on the two-component space (Re\([f]\), Im\([f]\)). Under time-reversal transformation, \( \eta \to \sigma^y \tau^y \lambda^x \eta. \)

The total gauge symmetry on \( \eta \) is the maximal subgroup of SO(8) that commutes with the spin-SU(2) operators. This is Sp(4) \( \sim \) SO(5) generated by the ten matrices \( \Gamma_{ab} = \frac{1}{2\sqrt{2}}[\Gamma_a, \Gamma_b] \), where

\[ \Gamma_1 = \sigma^y \tau^y \lambda^x, \quad \Gamma_2 = \sigma^y \tau^y \lambda^x, \quad \Gamma_3 = \tau^y \lambda^y, \]

\[ \Gamma_4 = \tau^x, \quad \Gamma_5 = \tau^x. \] (7.23)
These $\Gamma^a$ with $a = 1 \cdots 5$ define five gamma matrices that satisfy the Clifford algebra $\{\Gamma_a, \Gamma_b\} = 2\delta_{ab}$. $\Gamma_{ab}$ and $\Gamma_a$ are all $8 \times 8$ hermitian matrices. $\Gamma_{ab}$ are all antisymmetric and imaginary, while $\Gamma_a$ are symmetric.

A spin wave function can be constructed through a slave fermion wave function, by projecting the mean field ground state to satisfy the gauge constraints:

$$|G_{\text{spin}}\rangle = \prod_i P(\hat{n}_i = 2) \otimes P(\hat{\tau}^\mu_i = 0)|f_{a,a}\rangle.$$  \hfill (7.24)

Now let us consider the following mean field Hamiltonian of slave fermion on a honeycomb lattice:

$$H_{\text{MF}} = \sum_{\langle i,j \rangle} -t f_i^\dagger f_j + \sum_{\langle\langle i,j \rangle\rangle} i\lambda \nu_{ij} f_{i,a}^\dagger \tau^z_{ab} f_{j,b} + \sum_j i t' f_{j,a}^\dagger \tau^z_{ab} f_{j,b} + \sqrt{3} \hat{x} + \text{H.c.}$$  \hfill (7.25)

Written in terms of the Majorana fermion $\eta$, the mean field Hamiltonian reads:

$$H_{\text{MF}} = \sum_{\langle i,j \rangle} -t \eta_i^\dagger \Gamma_{12} \eta_j + \sum_{\langle\langle i,j \rangle\rangle} i\lambda \nu_{ij} \eta_i^\dagger \Gamma_5 \eta_j + \sum_j i t' \eta_j^\dagger \Gamma_4 \eta_{j+b} + \text{H.c.}$$  \hfill (7.26)

When $t' = 0$, this mean field Hamiltonian is a quantum “color” Hall Hamiltonian, i.e. it is equivalent to the Kane-Mele quantum spin Hall Hamiltonian \[5, 10\], although instead of a spin-orbit coupling, in Eq. 7.25 the $\lambda$ term is a color-orbit coupling. At the mean field level, the quantum color Hall mean field Hamiltonian Eq. 7.25 has edge states: there is a left-moving spin-1/2 doublet slave fermion with $\tau^z = 1$, and another right-moving spin-1/2 doublet slave fermion with $\tau^z = -1$. Backscattering between left and right moving slave fermions is forbidden, as long as the time-reversal symmetry and spin rotation symmetry are preserved. It is also easy to see that a spin-1/2 excitation is localized at the domain wall, consistent with the field theory discussed below Eq. 7.11.

The $t'$ term is a color-orbit coupling between 2nd neighbor sites along the $\hat{x}$ directions only. If $t' = 0$, the color-orbit coupling term $\lambda$ breaks the Sp(4) gauge symmetry down to its subgroup SO(4), which is generated by $\Gamma_{ab}$, with $a, b = 1, \cdots 4$; when $t'$ is nonzero, the gauge symmetry is broken down to SU(2) generated by $\Gamma_{ab}$, with $a, b = 1, 2, 3$. Since the $t'$ term is time-reversal even, when $t'$ is small compared with $t$ and $\lambda$, the edge state cannot be gapped out without degeneracy. Now the edge states can be describe by the following 1+1d field theory:

$$\mathcal{L} = \bar{\eta} \gamma_\mu (\partial_\mu - i \sum_{l=1}^3 A^l_\mu C^l) \eta + \cdots ,$$  \hfill (7.27)
Section 7.2. Lattice construction for $N = 2$, $m = 1$

where $A_{\mu}^I$ is the residual SU(2) gauge field, and $G^a = \epsilon_{abc} \Gamma^c$, $a, b, c = 1, 2, 3$. $\eta$ is the Majorana fermion introduced in Eq. [7.21]. $\gamma^0 = \tau^y$, $\gamma^1 = \tau^x$, $\gamma^5 = \tau^z$, $\bar{\eta} = \eta^t \gamma^0$.

Eq. [7.27] is precisely the same field theory that describes the spin-1/2 chain, if we take the standard SU(2) gauge field formalism for spin-1/2 systems [32]. There is no symmetry allowed fermion bilinear terms that can be added to Eq. [7.27]. It is well-known that spin-1/2 chain must be either gapless or degenerate, and when it is gapless it can be described by the 1+1d SU(2)$_1$ conformal field theory. Thus we conclude that the boundary of the bulk state Eq. [7.25] is either a gapless SU(2)$_1$ CFT, or degenerate due to spontaneous time-reversal symmetry breaking, which can be induced by a relevant four fermion term in Eq. [7.27].

It is well-known that the SU(2)$_1$ CFT (and spin-1/2 chain) is equivalent to an O(4) NLSM with a WZW term (Eq. [7.9]). The WZW term of Eq. [7.9] can be derived from Eq. [7.27] by coupling Eq. [7.27] to an unit-length O(4) order parameter:

$$\phi_0 \bar{\eta} \eta + \sum_{\mu=1}^{3} \phi^\mu i \bar{\eta} \gamma^5 S^\mu \eta,$$

where $S^\mu$ are the three matrices defined in Eq. [7.22] which generate the spin rotations. Careful analysis shows that the O(4) vector defined here has the same transformation as the O(4) vector in Eq. [7.9]. With the coupling in Eq. [7.28] after integrating out the slave fermions, a WZW term at precisely level-1 will be generated [187]. Thus this lattice construction is precisely consistent with the field theory analysis in the previous section.

In the bulk the slave fermion is gapped. Since the time-reversal symmetry in the bulk excludes the existence of a Chern-Simons term for the residual SU(2) gauge field, this non-abelian gauge field will lead to confinement, and this confined state has no topological degeneracy. At the boundary, the effect of this confinement is not totally understood. For instance, this confinement might gap out the boundary state through a spontaneous time-reversal symmetry breaking, namely the order $\langle \bar{\eta} \eta \rangle \neq 0$ is spontaneously generated. But nevertheless, the boundary will not be gapped out without degeneracy.

This lattice construction of SPT can be checked numerically in the future. Let us define the system on a torus without boundary, and a spin wave function can be constructed by gauge projecting the mean field state Eq. [7.25]. Given this projected spin wave function, one can numerically compute various quantities such as spin-spin correlation, topological entanglement entropy, and entanglement spectrum. Since the bulk is completely gapped, the spin correlation should be short ranged. And since the bulk of the system has no topological degeneracy, the topological entanglement entropy, which is defined as a universal constant term in addition to the standard area law, should be zero. However, since the system has nontrivial edge states, this edge states should also exist in the entanglement spectrum. We will leave these to future studies.
7.3 Discussion and Summary

In this work we studied a class of two dimensional symmetry protected topological phases with $\text{PSU}(N) \times \mathbb{Z}_2^T$ symmetry. These SPT phases are described by a 2+1 dimensional principal chiral model with $\Theta = 2\pi$ (Eq. 7.4), and their boundary states are described by a 1+1d NLSM with $\Theta' = \pi$, which must be either gapless or degenerate when the symmetry $\text{PSU}(N) \times \mathbb{Z}_2^T$ is preserved.

The principal chiral model Eq. 7.4 can describe some other symmetry protected topological phases as well. For example, the spin-2 AKLT phase on the square lattice is known to have a nontrivial 1d edge states. Unlike the 1d Haldane phase, AKLT states at higher dimensions require translation symmetry to protect its edge states. For example, on the square lattice, the edge states of the spin-2 AKLT phase is a spin-1/2 chain, and if the translation symmetry is broken, this edge spin-1/2 chain will be dimerized and gapped. The spin-2 AKLT phase on the square lattice can be viewed as a SPT phase with $\text{SO}(3) \times \mathbb{Z}_2$ symmetry, where the $\mathbb{Z}_2$ is translation by one lattice constant instead of time-reversal transformation. Then Eq. 7.3 and Eq. 7.4 with $\Theta = 2\pi$ can also describe the two dimensional AKLT phase, and its generalizations to arbitrary $N$. Our result and analysis apply for all even spatial dimensions. For large enough $N$ and $m$, $\pi_{2d+1}[\text{SU}(N)] = \mathbb{Z}$, and $\pi_{2d+1}[\text{U}(m) \times \text{U}(N-m)] = \mathbb{Z}_4$. Thus a SPT with $\text{PSU}(N) \times \mathbb{Z}_2^T$ symmetry exists in arbitrary even spatial dimension, and it is always described by a principal chiral model defined with order parameter $U$ introduced in Eq. 7.3.

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Part III

Weyl semimetal and its physics
Chapter 8

Possible topological phases of bulk magnetically doped Bi$_2$Se$_3$: turning a topological band insulator into the Weyl semimetal

The discovery of topological band insulators\cite{6,8,83} has been bringing attention to the topological properties of the band insulators. These phases are insulating in the bulk but support metallic surface states which is protected as far as the bulk gap remains open and time-reversal symmetry is respected. The topological properties of topological band insulators\cite{6,13,14} are guaranteed due to the well-defined bulk gap. However, it is demonstrated recently that gapless Weyl semimetal phase can also have topological protection to opening up a gap in bulk, edge-bulk correspondence, and gapless anomalous Hall response\cite{23,24,26,188}.

In this paper, we present that topological insulator materials can be turned into the Weyl semimetal phase upon doping the bulk with magnetic materials that is assumed to be ferromagnetically ordered. Then, the magnetization mass and topological band gap start to compete and result three phases including topological Weyl semimetal phase. The Weyl semimetal phase shows up when the magnetization mass is strong enough to close the topological band gap. This is striking in that in the previous studies on the effect magnetization (where magnetization mass is usually taken as the small ‘perturbation’), it is thought not desirable to close the band gap as it will destroy the topological properties of the topological band insulator and turn the material into trivial one. We hereby show that the strong magnetization mass in three-dimensional topological band insulator materials can generate a new topological phase; Weyl semimetal phase. The other two phases are topological band insulator phase (characterized by the axion angle $\theta = \pi$) and trivial insulator phase ($\theta = 0$). We show that the gapless Weyl phase is relatively easy to realize in the topological band insulator in experiment (See also the multilayered structure with topological insulators\cite{26} which uses the surface bands of topological insulators and recently proposed material HgCr$_2$Se$_4$\cite{188}),
compared to the complex compound structure \(\text{A}_2\text{Ir}_2\text{O}_7\) \cite{23, 25} where the possibility of realizing Weyl semimetal phase in condensed matter system is proposed. Our continuum theory for the Weyl semimetal phase is directly applicable to the well-known topological insulator Bi\(_2\)Se\(_3\)\cite{139}. Our work would be perhaps most relevant to the material TlBi(S\(_1-x\)Se\(_x\))\(_2\) where the gap could be tuned to the criticality in experiment\cite{143}. This continuum theory for the general low energy theory of the topological insulators is supported for the standard tight-binding model on the diamond lattice.

8.1 Theoretical Perspective

The universal low-energy physics of the topological insulator materials can be captured in the massive (isotropic) Dirac system

\[
H = v\tau^z \sum_{a=1}^{3} \sigma_a k^a + M(k)\tau^x
\]  

(8.1)  

where \(\tau^\mu\) and \(\sigma^\nu\) are Pauli matrices. We treat \(\sigma^\mu\) as the ‘real’ spin which is relevant in dealing with time-reversal symmetry. The Hamiltonian Eq.(8.1) incorporates with the two discrete symmetries: the time-reversal symmetry and the inversion symmetry. Usually, the Dirac mass \(M\) has the momentum dependence, i.e., \(M = M_0 + b k^2\) which can be tuned to be in the topological band insulator phase if \(M_0 b < 0\) and trivial phase if \(M_0 b > 0\)\cite{6}. When we are in the topological insulator phase\cite{6}, there is a single Dirac cone on the surface

\[
H_s = \pm v \sum_{i=1}^{2} \sigma^i \cdot k_i
\]  

(8.2)  

which can support a quantized anomalous Hall effect\cite{13} upon introducing time-reversal symmetry breaking gap \(\sim m\sigma^z\) on the surface. This effect attracts ennumerous attention\cite{140–142, 189} which is related to “axion electromagnetism”\cite{13, 14}. The effect can happen when the magnetization gap \(\sim m\) is safely smaller than \(M_0\) so that we are in the topological band insulator phase.

We further ask what would be the effect of the magnetization mass if it turns large enough (due to the bulk magnetic impurity doping). We assume that the magnetic material doped in the topological band insulator forms a ferromagnetic order to supply the necessary mass. If this magnetization is large enough, then strikingly it can generate a gapless Weyl semimetal phase. To study this, we introduce the magnetization mass in the form of

\[
H_m = Jm \cdot \sigma \tau^0
\]  

(8.3)  

to the Hamiltonian Eq.(8.1). Due to the isotropy in our model, we can further simplify \(Jm = m\hat{z}\) (redefining \(Jm \rightarrow m\)). As a whole, we will deal with the Hamiltonian

\[
H = v\tau^z \sum_{a} \sigma_a k^a + M(k)\tau^x + m\sigma^z\tau^0
\]  

(8.4)
which supports three phases: topological band insulator with time-reversal symmetry broken surface, Weyl semimetal phase, and trivial phase (without losing generality, we choose $M_0 > 0$ and $m > 0$). We will show that the transition between two insulating phases and gapless Weyl semimetal phase happens at $M_0 = m$.

Upon with this general consideration, we start to discuss the details of the Hamiltonian with the bulk magnetization mass Eq. (8.4).

- **Energy spectrum of the band theory:** The general behavior of the spectrum of the Hamiltonian Eq. (8.4) can be easily read off from the following commutation relations

![Figure 8.1: Proposed phase diagram in terms of $(m, M)$ for $b < 0$ in Hamiltonian Eq. (8.4): (A),(B) Topological band gap $M$ is larger than magnetization mass $m$, thus we are in the insulating phase. We have a topological band insulator (A) for $M > 0$ and trivial insulator (B) for $M < 0$. (C),(D) Magnetization mass is stronger than the topological band gap, and we have a Weyl semimetal phase. Note that if $m \rightarrow -m$, then two Weyl points change the sign of the chirality. At the transitions $|m| = |M|$, two Weyl points meet each other and result topological or trivial insulators.](image-url)
\[ \sigma^z \tau^0, \tau^x \] \neq 0. Due to the commutation \([\sigma^z \tau^0, \tau^x] = 0\), we will have the competition between the magnetization mass \(m\) and the topological mass \(M_0\). Explicitly, we have the energy spectrum \(E(k)\) for general \(m\) and \(M(k)\)

\[
E(k) = \pm \sqrt{v^2(k_x^2 + k_y^2) + (m \pm \sqrt{M^2 + v^2k_z^2})^2}
\]  

(8.5)

we find that there are two mass gaps \(\Delta_{\pm}\) where \(\Delta_{\pm} = m + \sqrt{M^2 + v^2k_z^2}\) and \(\Delta_{\pm} = m - \sqrt{M^2 + v^2k_z^2}\). We immediately see that the gap \(\Delta_{\pm}\) can close if \(m > M_0\) at the momentum \(vk_z = \pm \sqrt{m^2 - M(k)^2}\) which are the positions of Weyl points in the momentum space. We now discuss two cases where \(m < M_0\) and \(m > M_0\) (See Fig[8.1]).

- **Topological band and trivial insulator phases:** Here we discuss the case \(m < M_0\). To study these phases, we use the adiabatic argument, i.e., we are in the same topological class as far as the gap remains open at \(k = 0\) (we assume that \(k = 0\) point is the only point which possibly closes the band gap) and the inversion symmetry is protected. As \(\Delta_{\pm}\) is always positive for any \(m\), our main focus goes to \(\Delta_{-}\). The Dirac mass \(\Delta_{-}(k = 0) = m - M_0\) which closes at \(m = M_0\), signaling quantum phase transition to the Weyl semimetal phase. When \(m < M_0\), we need to further specify the mass \(M(k) = M_0 + bk^2\) and have a topological band insulator phase due to the band inversion if \(M_0b < 0\) and a trivial insulator phase if \(M_0b > 0\).

When we are in the topological band insulator phase (and also the chemical potential lies in the surface magnetization gap \(\sim m < M_0\)), we have Chern-Simon effective surface theory with external electromagnetic gauge \(A_{\mu}\)

\[
L_{\text{eff}} = \frac{|m|}{2m} \times \frac{1}{4\pi} A_\mu \partial_\nu A_\lambda \varepsilon^{\mu\nu\lambda}
\]

(8.6)

which is the quantum anomalous Hall effect with the quantized hall coefficient \(\sigma_{xy} = \pm e^2/2h\).

- **Gapless Weyl semimetal phase:** We now proceed to the case \(m > M_0\) where the mass \(\Delta_{-}(k = 0) < 0\). For the low-energy physics, we ignore the quadratic dependence on \(M(k) = M_0 + O(k^2)\) to clarify the physics of this phase. Then, we have two Dirac nodes in \(O(k)\) where \(vk_z = vK_{c,\pm} = \pm vK_c = \pm \sqrt{m^2 - M_0^2}\). Near the critical points \(k_{c,\pm} \sim \pm K_c\), the low-energy theory of the Hamiltonian Eq.(8.4) reduces into (with \(q_{z,\pm} = k_z - K_{c,\pm}\))

\[
H(k) = \epsilon(K_c) + \begin{bmatrix}
  u_+ q_{z,\pm} & v & vk_+ \\
  v & -u_+ q_{z,\pm} & -v
\end{bmatrix}
\]  

(8.7)

with anisotropic Dirac speed along \(\hat{z}\) direction, \(u_\pm = \mp v^2|K_c|/m\). This Hamiltonian is nothing but the Weyl fermion with the winding number \(\pm 1\) localized at \(K_{c,\pm}\) (two Weyl points carry the chirality \(c_{\pm} = \text{sign}(u_\pm) = \mp 1\) at the Dirac point[23]).

Due to this non-zero winding number, the Weyl Hamiltonian Eq.(8.7) has an anomalous Hall effect[24, 26, 188] in xy-plane. Because each layer of the whole bulk participates in anomalous Hall effect, we define the anomalous Hall response per layer. The simple computation shows that the first chern number \(C_{k_z} = \pm 1\) for \(k_z \in (-K_c, K_c)\) with \(K_c = |K_{c,\pm}|\).
Then, this would support the anomalous Hall conductance (when the chemical potential is exactly at the Dirac point)

\[ \sigma_{xy} = \frac{e^2}{2\pi\hbar} 2K_c \]  

(8.8)

This effect can be defined up to modular \( e^2/\hbar \) due to the ambiguity\[24, 26\] in \( |K_c| \) which is up to modular \( \pi \) (half of the size of the reciprocal vector along \( \hat{z} \)).

When two Weyl points are brought to the Brillouin zone center and pair-annihilate\[23\] \( (m \to M_0) \), we have topological insulator phase (characterized by axion angle \( \theta = \pm\pi \)) or trivial insulator phase \( (\theta = 0) \). The two axionic response of the resulting insulator phases can be anticipated from the inversion symmetry encoded in Eq. (8.1) and Eq. (8.4) because the angle \( \theta \to -\theta \) under the inversion. By noting the following two reasonings (1) the axion angle \( \theta = \pm\pi \) \( (\theta = 0) \) for topological insulator phase (trivial insulator phase) at \( m \to 0 \) and (2) the angle is tied to topological structure of the band structure \[190, 191\] and thus cannot be changed smoothly as far as the gap remains open, we conclude that the full region of topological band insulator (trivial insulator) phase in the phase diagram is characterized by \( \theta = \pm\pi \) \( (\theta = 0) \). If the inversion symmetry is broken down, then the axion angle \( \theta \) is no longer protected and expected to be continuously varying in terms of the parameters of the system.

It is also interesting to note that we can realize quantized layered anomalous Hall effects if the two Weyl points are dragged \( (K_c = \pi) \) to the Brillouin zone boundary\[26\] and pair-annihilated. Then each layer in the bulk carries the Hall conductance

\[ \sigma_{xy} = \frac{e^2}{\hbar} \]  

(8.9)

and each layer forms integer quantum Hall states without magnetic field. From this consideration, we could remarkably obtain various interesting known topological phases, topological band insulator (gapped), Weyl semimetal phase (critical), and three-dimensional anomalous Hall (gapped) phase, within the single effective theory of the topological band insulator. In fact, we can go further if we notice that the same Hamiltonian can describe the two-dimensional topological band insulator. When the sample width of the three-dimensional topological insulator is reduced, then the material turns into the two-dimensional topological band insulator\[192\] (with some oscillatory behavior as the function width). Furthermore, it is known that the two-dimensional topological insulator materials can be turned into the anomalous Hall effect upon doping of the magnetic materials\[140–142, 189\]. Hence, it is plausible to connect the three-dimensional Weyl semimetal phase to the two-dimensional anomalous Hall effect in the sense of the dimensional cross-over\[192\].

- **Other commuting masses and possible gapless phases**: The realization of Weyl semimetal phase in this paper rely on the commutation relation between mass/kinetic terms in Hamiltonian Eq. (8.4). In general, if two Dirac masses \( Q \) and \( M \) satisfy \([Q, M] = 0\), then two masses tend to kill each other. Given the topological mass \( M \sim \tau^z \) and the kinetic term \( K \sim \tau^z \sigma^a \) in Eq. (8.4), we can classify the mass terms \( Q \) that gives the possible gapless
phases from the topological band insulator. The conditions are \([Q, M] = 0\) and \([K_i, Q] \neq 0\) for at least one of \(i = 1, 2, 3\). Then these conditions include \(Q = (\hat{m} \cdot \hat{\sigma}) \tau^0\) which generates ‘two’ Weyl points, and \(Q = \tau^x \sigma_i\) which generates a gapless cylinder around the origin, e.g., \(k_x^2 + k_y^2 = k_c^2\) along \(k_z\) for \(Q = \tau^x \sigma^z\). However, the second case would be easily gapped out in perturbation. So the magnetization mass is the only mass that is capable of inducing the Weyl semimetal phase in competition with the topological band gap. However if there is an additional lattice symmetry, then the gapless cylinder resulting from \(Q\) may end up with multiple of Weyl nodes which are protected to be gapless by certain lattice symmetries \([26]\).

### 8.2 On real material

We begin with the basic model for \(\text{Bi}_x \text{Sb}_{1-x}\) with the magnetic mass due to the Zeeman coupling \(\sim J \hat{m} \cdot \hat{S}\) where \(\hat{m}\) is the polarized magnetic moment in the system. Even though \(\hat{m}\) can polarize in any direction, we further assume \(\hat{m}\) to be parallel with \(\hat{z}\). This can be prepared by applying the external magnetic field in \(\hat{z}\) when the magnetic order sets into the sample. So, we assume \(m_{x,y} << m_z = m\) and further ignore \(m_{x,y}\). We begin with the standard tight-binding model on the diamond lattice\([6]\) for the topological band insulator

\[
H_{TI} = t \sum_{<i,j>} c_i^\dagger c_j + i \lambda_{SO} \sum_{<<i,j>>} c_i^\dagger \hat{s} \cdot \hat{e}_{ij} c_j \tag{8.10}
\]

where the second term encodes the spin-orbit coupling which connects the next nearest neighbors. The Hamiltonian has the inversion symmetry and time reversal symmetry. The spectrum of the Hamiltonian Eq.(8.10) is very well understood and is topological band insulator (with the distortion). Now, we introduce the magnetization over the sample and assume that the doped magnetic material approximately induces the uniform on-site Zeeman term

\[
H_z = m \sum_i c_i^\dagger s^z c_i \tag{8.11}
\]

We move to the momentum space for the Hamiltonian \(H_{TI} + H_z\) and find

\[
H = \sum_{i=1}^5 \Gamma_i \Gamma^i + m \Gamma^{34} \tag{8.12}
\]

where we followed the notation of Fu et.al.\([6]\) We can diagonalize it to obtain the band structure

\[
E(k) = \pm \sqrt{d_3^2 + d_4^2 + (m \pm \sqrt{d_1^2 + d_2^2 + d_5^2})^2} \tag{8.13}
\]

Note the remarkable resemblance of the above energy spectrum Eq.(8.13) to the band spectrum Eq.(8.5) which we obtained from the continuum model. As \(H_z\) is independent of the momentum \(k\), we don’t need to solve for all momentum \(k\) but we can simply look at the
points where the gap for $H_{TI}$ Eq.(8.10) is small and where $d_3(k), d_4(k)$ and $d_5(k)$ go as $\sim |k| + O(k^2)$. There are eight such points (Γ point, three $X$ points, and four $L$ points) in the Brillouin zone and we will have Weyl points out of these eight points. For example, we find that there are two Weyl points near the Γ point if $m > m_c = \sqrt{m^2 - (4t)^2}$ at

$$k_c = (0, 0, \pm \sqrt{\frac{m^2 - (4t)^2}{t^2}}) \quad (8.14)$$

where $|4t|$ is the band gap at the Γ point. We find that this simple tight-binding model agrees with the continuum calculation, and hence we’ve provided that the microscopic lattice model for the Weyl phase.

- **experimental preparation**: In the experiment, topological band gap $M$ tends to be the largest energy scale in the system ($\sim 0.3$eV for Bi$_2$Se$_3$[139]) and this would act as the drawback to realize the Weyl semimetal phases in that the magnetization mass $m$ should win against the band gap $M$. Hence it is desirable to reduce the band gap by bringing the system to near the critical point ($M \to 0$) between topological and trivial insulators. Recently, the mass gap of the topological insulator material TlBi(S$_{1-x}$Se$_x$)$_2$ appears to be under the control and could be tuned to the criticality in experiment[143]. Though it is difficult to predict the energy scale for the magnetic mass, some theoretical calculations ($\sim 5 - 50$meV) and experiments ($\sim 0.1$eV) seems to be positive[140, 189] to see this physics (at least in the thin film limits). Due to the disorders, it might not be easy to detect the transition itself. However, if the magnetic mass is large enough, Weyl phase should appear. If there are more than one Dirac point in the low energy, there could be more than two Weyl points (depending on the precise form of the ‘representation’ of the magnetization mass at the Dirac point).

In terms of observation, the best way to detect Weyl semimetal phase would be perhaps ARPES experiment to see the Weyl points and the strange surface states. Transport experiment would be also applicable to detect anomalous Hall effects. Note that $\sigma_{xy} \sim k_c \sim (m^2 - M^2)^{1/2}$ where $M$ is tunable by controlling the width of the quantum well. Via this, $\sigma_{xy}$ would be tunable in the thin film limit. For the reasobale prediction with the magnetization gap $\sim 50$meV in thin film limit and the optimal preparation of the sample $M_0 \to 0$, we predict $\sigma_{xy} \sim O(10^4) \Omega^{-1} \text{cm}^{-1}$.

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Chapter 9

Superconductivity of doped Weyl semimetals: finite-momentum pairing and electronic analogues of the $^3\text{He}-\text{A}$ phase

Recent progress in our understanding of non-interacting Bloch electrons reveals a large class of gapped topological phases, the so-called topological insulators and superconductors. For example, a time-reversal-symmetric topological insulator is a band insulator that cannot be continuously tuned into a trivial atomic insulator, as long as time-reversal symmetry is respected. A topological insulator is featured by a single Dirac cone in its surface state spectrum. Typically, these topological phases are realized in systems with strong spin-orbit coupling. It is known that when topological insulators are combined with superconductivity via the proximity effect or via phonon-mediated attractive interaction, the interesting interplay between electron pairing and the spin-orbit coupling results in exotic superconductivity. For instance, when a topological insulator is doped and turned into a superconductor, an odd-parity topological superconductor is obtained with a single gapless Majorana surface state, which is protected by time-reversal symmetry.

Another type of gapless ‘topological matter’, the Weyl semimetal, is currently being studied intensively and is proposed to be realized in experiments. Its electronic structure has an even number of Weyl nodes – two cylindrical 3D cones that touch at their apex, the Weyl point – which carry non-trivial winding numbers ensuring their stability. These Weyl nodes can be thought of as 3D analogs of the two component Dirac fermions in graphene and at the surface of a 3D topological insulators. They exhibit spin-momentum locking and thus require strong spin-orbit coupling to be realized. In analogy with superconductivity in topological insulators, it is natural to expect interesting superconducting states to emerge in these systems upon doping, resulting from their non-trivial topological winding numbers. To realize a Weyl semimetal phase requires either time-reversal...
symmetry\cite{23} or inversion symmetry\cite{196} to be broken. In this paper we concentrate on the inversion-symmetric case, in which the two nodes connected by the inversion symmetry carry opposite chirality. Upon slight doping there are at least two disconnected components to the Fermi surface around the nodes, shifted in momentum space from the inversion-symmetric high-symmetry points such as the Γ-point. We will show that the interplay between the finite-momentum displacement and the non-trivial winding numbers around each Weyl node leads to interesting superconducting states.

The finite momentum shift of the Fermi surface motivates the study of finite-momentum pairing states or Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) states\cite{197, 198}. FFLO states break translational symmetry and have interesting physical properties\cite{197, 199}. In the Weyl semimetals, the center of momentum of the FFLO pairs is fixed by the momentum of the Weyl nodes. Similarly, the non-trivial winding around the nodes and the broken time-reversal symmetry suggests the possibility of realizing even/odd-parity BCS states that are electronic analogues of the $^3$He-A phase\cite{200, 201}. Since the $^3$He-A phase has nodes with non-trivial winding number which guarantees the existence of a dispersionless surface states\cite{201}, the Weyl semimetal in these phases is also expected to support zero-energy surface flat bands, similar to a Weyl semimetal in proximity to a superconductor\cite{201, 204}.

Surprisingly, when the attractive interaction is completely local in real space and represents a phonon-mediated interaction, we find from a self-consistent mean field calculation that the fully-gapped finite-momentum pairing is energetically favored over the even-parity BCS state (both pairing states can be thought of as spin-‘singlet’ pairings though ‘singlet’ is not a very exact terminology since spin-rotational symmetry is broken) and is stable against weak disorder. Hence, there is a good chance of experimentally observing these exotic phases. To be concrete, we concentrate on a specific lattice model realizing an inversion-symmetric Weyl semimetal and solve the gap equation of the lattice model in the BCS approximation. We also discuss the applicability of our result to other models realizing Weyl semimetals.

The proximity effect of an s-wave superconductor on an undoped Weyl semimetal has been studied by Meng and Balents in Reference\cite{202}. In contrast to this work, where the superconductivity is extrinsic, we are interested in the intrinsic superconductivity of the doped Weyl semimetal. Note that if the Weyl semimetal is undoped, the intrinsic superconducting gap and the critical temperature are expected to be vanishingly small since the density of states goes to zero at the Weyl point.

\section{Model}

The model we consider in this work is given by the Hamiltonian

$$H = H_0 + V_{ee} \quad (9.1)$$
where $V_{ee}$ is an electron-electron interaction term to be specified below. For the kinetic term, $H_0$, we take the minimal two-band lattice model\cite{24}:

$$
H_0 = t(\sigma^x \sin k_x + \sigma^y \sin k_y) + t_z(\cos k_z - \cos Q)\sigma^z + m(2 - \cos k_x - \cos k_y)\sigma^z - \mu.
$$

This model realizes a Weyl semimetal with two Weyl points at momenta $\vec{P}_\pm = (0, 0, \pm Q)$. $\sigma^x,y,z$ are the Pauli sigma matrices (for later use we define $\sigma^0$ to be the $2 \times 2$ unit matrix), $t$ and $t_z \sin Q$ are the Fermi velocities at the Weyl points in the $x,y$ and $z$ directions respectively. Without a loss of generality, we assume $t = t_z \sin(Q)$ such that the Fermi velocity around the Weyl points is isotropic. We have explicitly included the chemical potential $\mu$ in the kinetic term. We are primarily interested in the parameter range $0 < |\mu/t| \ll Q$, when the Fermi surface consists of two disconnected spherical components around the Weyl points (see Fig. 9.1). In this case, the states on the Fermi surface have spin-momentum locking similar to the surface states of a strong topological insulator. This property will play an important role in our discussion of pairing states below.

The electron-electron interaction is short ranged and takes the form

$$
V_{ee} = V_0 \sum_i n_i n_i + V_1 \sum_{\langle ij \rangle} n_i n_j = \sum_{\vec{k}} V(\vec{k}) n_{\vec{k}} n_{-\vec{k}},
$$

where $n_i = \sum_\sigma c^\dagger_{i,\sigma} c_{i,\sigma}$ is the number of electrons on site $i$, and the second sum is over nearest neighbors only. $V(\vec{k}) = V_0 + V_1(\cos k_x + \cos k_y + \cos k_z)$ is the Fourier transform of the real-space interaction. $V_0$ represents a phonon-mediated attractive on-site interaction and $V_1$ the nearest-neighbor interaction. We are mainly interested in the case $V_0 < 0$ and $|V_0| \gg |V_1|$ when electrons form Cooper pairs and condense. The phenomenological interaction term \cite{9.3} captures the tendency of $d$-wave pairing for $V_1 < 0$ and $V_0 > 0$ in the context of high-Tc superconductors such as cuprates\cite{205}.

The point group symmetry of the model Hamiltonian, $H$, is $C_{4h} = \{I^\mu C^\eta_4 | \eta_1 = 0, 1; \eta_4 = 0, 1, 2, 3\}$, where

$$
I : \sigma^z H(-\vec{k})\sigma^z = H(\vec{k}),
$$

$$
C_4 : S^\dagger H[R_{\pi/2}(\vec{k})]S = H(\vec{k}),
$$

with $S = \frac{1}{\sqrt{2}}(\sigma^0 + i\sigma^z)$ and $R_{\pi/2}$ a rotation by an angle $\pi/2$ around the $z$-axis. $I$ is the inversion symmetry that takes $\vec{r} \rightarrow -\vec{r}$. Each spatial rotation is accompanied by an equal spin rotation, manifesting the spin-momentum locking due to the presence of strong spin-orbit coupling. The $C_4$-rotation symmetry in the $xy$-plane is not required to realize a Weyl semimetal, but is present in this model and similar lattice rotations are present in other models we discuss later.

To make a connection to previous work\cite{23, 24, 26, 27} and to obtain a general understanding of Weyl semimetal phases, we derive the low energy effective theory corresponding
to the lattice model (9.1). Expanding $H(\vec{k})$ in the small momentum $\vec{q} = \vec{k} - \vec{P}_\pm$ around the two Weyl Points denoted by $\pm$, we obtain

$$H_0 = \sum_{\vec{k}} c^\dagger(\vec{k})H_0(\vec{k})c(\vec{k}) \approx \sum_{a=\pm} \psi^\dagger_a(\vec{q})h_a(\vec{q})\psi_a(\vec{q}). \quad (9.5)$$

The effective kinetic Hamiltonian $h_\pm(\vec{q})$ is given by

$$h_\pm(\vec{q}) = t(q_x\sigma^x + q_y\sigma^y \mp q_z\sigma^z) - \mu. \quad (9.6)$$

Similarly, we obtain for the interaction term

$$V_{ee} = \sum_{\vec{k},\vec{p},\vec{q}} V^{abcd}_{\vec{k},\vec{p},\vec{q}}(\vec{q})\psi^\dagger_{a,\sigma}(\vec{k})\psi^\dagger_{b,\tau}(\vec{p} - \vec{q})\psi_{c,\tau}(\vec{p})\psi_{d,\sigma}(\vec{p}), \quad (9.7)$$

where roman letters denote the nodal indices $\pm$ and $\sigma, \tau$ are spin indices. Here and henceforth, repeated indices are summed over. In the BCS channel (see App. 12.1 for details)

$$V_{ee} = \sum_{\vec{k},\vec{l}} V^{abcd}_{\vec{k},\vec{l}}(\vec{q})\psi^\dagger_{a,\sigma}(\vec{k})\psi^\dagger_{b,\tau}(\vec{l})\psi_{c,\tau}(\vec{p})\psi_{d,\sigma}(\vec{l}), \quad (9.8)$$

with

$$V^{+:+:-} = V^{-:-:+} = V_0 + 3V_1 - \frac{1}{2}(\vec{k} - \vec{l})^2,$$

$$V^{+:+:+} = V_0 + V_1 + V_\perp + V_\parallel^+, \quad (9.9)$$

$$V^{+:-:-} = V_0 + 2V_1 + V_\perp + V_\parallel^-, \quad V_\perp = -\frac{1}{2}(\vec{k}_\perp - \vec{l}_\perp)^2,$$

and

$$V_\parallel^+/V_1 = [1 - \frac{1}{2}(k_z - l_z)^2] \cos 2Q + (k_z - l_z)\sin 2Q,$$

$$V_\parallel^-/V_1 = [1 - \frac{1}{2}(k_z - l_z)^2] \cos 2Q - (k_z - l_z)\sin 2Q,$$

where $\vec{k}_\perp = (k_x, k_y, 0)$. These expressions will be used in the next section.

**9.2 Mean field theory and pairing channels**

We treat the interaction term $V_{ee}$ in a mean field approximation and solve the resulting gap equations self-consistently. In addition to the more standard BCS pairing, we also study finite-momentum or FFLO pairing.
Figure 9.1: (Color online) A schematic diagram of the spin texture around the Weyl nodes in momentum space and the pairing states. (a) The spin direction of the eigenstates is given by thick arrows. The double-headed arrows labeled with (1) and (2) indicate the partner states in the BCS pairing. The spin state is maximally anti-parallel for (1) and parallel for (2), indicating that there will be nodes in the latter case if the pairing is in the singlet channel. Contrary to the BCS pairing, the FFLO pairing (3) connects two states within the same node ('intra-nodal' pairing). The two states connected by the FFLO pairing have the opposite spin directions. (b) Position of the nodes for the even-parity state. The nodes of the same chirality are on the same component of the Fermi surface, with their partner nodes of opposite chirality on the other. The filled circle represents a node of chirality +1 and the crossed circle represents a node of chirality −1. Hence, there are four nodal points on the Fermi surface of the even-parity paired BCS state.
9.2 Mean field theory and pairing channels

The symmetry classification of different BCS pairing order parameters in a doped Weyl semimetal, according to the lattice symmetry (9.4), is summarized in Table 9.1 (see App. 12.3 for more details). There are three fully-gapped BCS pairing order parameters ($\Gamma_1$ and $\Gamma_3^\pm$) and one that has nodal lines ($\Gamma_2$).

In the continuum theory, the pairing terms of Table 9.1 take the form

$$\sum_{\vec{k}} \Delta_{\sigma\tau}(\vec{k}) c_{\sigma}^\dagger(\vec{k}) c_{\tau}^\dagger(-\vec{k}) \approx \sum_{\vec{q}} \Delta_{a,b}^{ab}(\vec{q}) \psi_{a,\sigma}^\dagger(\vec{q}) \psi_{b,\tau}^\dagger(-\vec{q}),$$

(9.11)

The standard BCS pairing term connects two Weyl nodes in the effective theory. The explicit form of $\Delta_{a,b}$ and $\Delta_{\sigma\tau}$ can be found in Table 9.1 and in Eq. (12.6) in App. 12.1. The self-consistent gap equation takes the form

$$\Delta_{a,b}(\vec{p}) = \sum_{\vec{k}} V_{a,b,c,d}(\vec{p} - \vec{k}) \langle \psi_{c,\tau}(-\vec{k}) \psi_{d,\sigma}(\vec{k}) \rangle,$$

(9.12)

where the expectation value is taken with respect to the mean field superconducting state (see App. 12.1 for more explicit expressions for the gap equations).

9.2.2 FFLO pairing

In the doped Weyl semimetal, the Fermi surface is formed around the Weyl points $\vec{P}_\pm$, and it is natural to expect a finite-momentum pairing to compete with the standard BCS-paired states. We therefore introduce a FFLO state with a center of momentum at $2\vec{P}_\pm$, which pairing function satisfies

$$\Delta_{FFLO}(\vec{r}) \propto \exp(2i\vec{P}_+ \cdot \vec{r}) \pm \exp(2i\vec{P}_- \cdot \vec{r})$$

(9.13)
Mean field theory and pairing channels  

Table 9.2: Classification of the FFLO states of superconducting Weyl fermions based on the lattice symmetry $C_4$. The notation is the same as in Table 9.1. We assume that the center of momentum for the pairing is at $\vec{P}_\pm$. Note that the symmetry is only $C_4$ on the $xy$-plane without the inversion because ‘inversion’ is already encoded by the ansatz Eq. (9.13). This classification is essentially the same as that of BCS-type pairing order parameters.

The self-consistent equations for these pairing order parameters take the form

$$
\Delta_{\sigma\tau}(\vec{p}, \pm \vec{P}) = \sum_{\vec{k}} V(\vec{p} - \vec{k}) \langle \psi_{\pm,\tau}(-\vec{k}) \psi_{\pm,\sigma}(\vec{P}) \rangle,
$$

where the two nodes $\pm$ are decoupled. These FFLO states correspond to the intra-node pairing, in contrast to the BCS case which is inter-node pairing (see Fig. 3.1). The two states of the pairings $\Delta_{\pm}^{FFLO}$ in Eq. (9.13) with a relative phase of $\pm 1$ between the two components of the Fermi surface have the same mean field energy since the two nodes are decoupled in the mean field theory.

9.2.3 Mean field energy

Having identified the possible superconducting states, we compute their free energy by solving the self-consistent gap equations numerically. We are interested in the case $|V_0| \gg |V_1|$ with $V_0 < 0$ where the spin singlet is preferred. We denote the pairing term $\propto i\sigma^y$ in Table 9.1 as ‘singlet’ and the other terms $\propto i\vec{\sigma}\sigma^y$ as ‘triplet’. The singlet and triplet components have a different dependence on the interaction parameters $V_0$ and $V_1$. The gap of the triplet components depends only on the value of $V_1$, while the singlet component depends only on $V_0 + 3V_1 \approx V_0$ or $V_0 + V_1(5 + \cos 2Q)/2 \approx V_0$. We therefore consider in the following only the singlet component $\propto i\sigma^y$ of $\Gamma^1$ for the BCS and FFLO states.

For these two states the BCS mean field approximation is

$$
H = H_0 + V_{ee}^{\text{pair}},
$$

where $H_0$ is given by Eq. (9.2) and $V_{ee}^{\text{pair}}$ is the effective projected pair potential derived from
the lattice interaction in Eq. (9.3). For the $\Gamma^1$-BCS state we have

$$V_{ee}^{\text{pair}} = -U_{\text{BCS}} \sum_{\vec{k}, \vec{p}} P_{\vec{k}}^I P_{\vec{p}},$$

$$U_{\text{BCS}} = V_0 + V_1 \frac{5 + \cos(2Q)}{2},$$

$$P_{\vec{k}}^I = \psi^I(\vec{k}) \tau^x i \sigma^y \psi^*(-\vec{k}),$$

and the gap equation is

$$\Delta = -\frac{U_{\text{BCS}}}{4} \int \langle \psi_{a,\alpha}(\vec{k})(\tau^x)^{ab}(-i \sigma^y)^{\alpha\beta} \psi_{b,\beta}(\vec{k}) \rangle.$$ (9.17)

For the $\Gamma^1$-FFLO state we obtain

$$V_{ee}^{\text{pair}} = -U_{\text{FFLO}} \sum_{\vec{k}, \vec{p}} P_{\vec{k}}^I P_{\vec{p}},$$

$$U_{\text{FFLO}} = V_0 + 3V_1,$$

$$P_{\vec{k}}^I = \psi^I(\vec{k}) i \sigma^y \psi^*(-\vec{k}),$$

with a gap equation

$$\Delta = -\int \frac{U_{\text{FFLO}}}{2} \langle \psi_{a,\alpha}(\vec{k})(\sigma^y)^{\alpha\beta} \psi_{a,\beta}(\vec{k}) \rangle.$$ (9.19)

In this standard BCS-type approximation, we can evaluate the energy $E$ of the pairing states with the pairing amplitude $\Delta_{\vec{k}} = -U \langle P_{-\vec{k}} \rangle$ (with the effective pairing interaction strength $U$) by computing

$$E = E_{\text{el}} + E_{\text{sc}},$$

$$E_{\text{el}} = \sum_{\vec{k} \in d\Omega, \epsilon_\text{sc} < 0} \epsilon_\text{sc}(\vec{k}) n_e[\epsilon_\text{sc}(\vec{k})] - \sum_{\vec{k} \in d\Omega, \epsilon_\text{fs} < 0} \epsilon_\text{fs}(\vec{k}) n_e[\epsilon_\text{fs}(\vec{k})],$$

$$E_{\text{sc}} = -\sum_{\vec{k} \in d\Omega} \frac{\Delta_{\vec{k}} \Delta^*_{-\vec{k}}}{2U} + h.c.$$ (9.20)

Here $n_e$ is the filling of the electron for the state at $\vec{k}$ of energy $\epsilon(\vec{k})$, $\epsilon_\text{sc}$ is the energy of the filled band of the BdG quasiparticle with mean field gap $\Delta$, and $\epsilon_\text{fs}$ is the energy of the filled bands of the free Weyl electrons without pairing, i.e. the energy of the normal state. Thus, the second line of Eq. (9.20) represents the energy gain of the superconducting state relative
to the normal state by opening up a gap near the Fermi surface. The last line of Eq. (9.20) represents the contribution from the pairing interaction labeled by the momentum $\vec{k}$. The range of the summation is restricted to a shell $d\Omega$ around the Fermi surface, which width is determined by the strength of the attractive interaction.

In Fig. 9.2 we plot the mean field energy for the two parings, as obtained from Eq. (9.20), as a function of the interaction strength $V_0$. The $\Gamma^1$-FFLO state has a larger gap than the $\Gamma^1$-BCS state and is energetically favored. This result can be understood by considering the spin-momentum locking around the Fermi surface. For the even-parity pairing state, the state $|\vec{k}, \alpha\rangle$ ($\alpha$ is the spin state) is paired with the inversion partner state $|-\vec{k}, \sigma^z\alpha\rangle$. The pairing amplitude is of the form $\sim \langle c^\dagger(\vec{k})i\sigma^y c^*(\vec{k}) \rangle$ which takes the maximum value if the two states at $\vec{k}$ and $-\vec{k}$ have opposite spins. However, the spins at $\vec{k}$ and $-\vec{k}$ are not anti-parallel and even become parallel at the poles (which is the origin of the nodes, see Fig. 3.1) which tends to reduce the superconducting gap. In contrast, the FFLO state connects the states $|\vec{k} + \vec{Q}, \alpha\rangle$ and $|-\vec{k} + \vec{Q}, \beta\rangle$ via the spin singlet channel with $\beta = -\alpha$ (anti-parallel spins). A gap opens up everywhere at the Fermi surface with a larger gap than the even-parity BCS state. This is very similar to the surface of topological insulator which we discuss Appendix B (See also Reference [206]. The similar finite-momentum pairing (“intra-valley” pairing or “Kekule” pairing) can happen in a graphene in the presence of a nearest-neighbor attractive interaction [207, 208].

9.3 Discussion

In this section, we discuss the nodal structure of the $\Gamma^1$-BCS state and the effect of the disorder on the $\Gamma^1$-FFLO state. Like in the last section, we consider only the singlet components of these states, assuming $|V_0| \gg |V_1|$.

9.3.1 $\Gamma^1$-BCS state

The pair potential term in the mean field Hamiltonian of the singlet component of the $\Gamma^1$-BCS state is

$$H_{\text{pair}}^{\text{BCS}} = \sum_{\vec{k}} \Delta c_{\alpha}^\dagger(\vec{k})(i\sigma^y)^{\alpha\beta} c_{\beta}^\dagger(-\vec{k}) + \text{h.c.}$$  \hspace{1cm} (9.21)

$$= \sum_{\vec{q}} \Delta \psi_{a,\alpha}^\dagger(\vec{q})(r^x)^{ab}(i\sigma^y)^{\alpha\beta} \psi_{b,\beta}^\dagger(-\vec{q}) + \text{h.c.}$$

The second form is obtained in the low energy theory. This superconducting state is an even-parity state and has four point nodes on the Fermi surface at $q_x = q_y = 0$ and $q_z = \pm \sqrt{\Delta^2 + \mu^2}$ (see Fig. 3.1). The gap remains closed even when the triplet pairings of the $\Gamma^1$-BCS state in Table 9.1 are included.
Figure 9.2: (Color online) mean field energy $E$ of the even-parity $\Gamma^1$-BCS and the $\Gamma^1$-FFLO states as a function of interaction strength $V_0$. Other model parameters used to obtain this plot are $\mu/t = 0.3$, $Q = 0.7$, $V_1 = 0$, and $d\Omega = 0.2$.

The two nodal points near Weyl node $\vec{P}_+$ ($\vec{P}_-$) carry a winding number of +1 (-1). To demonstrate this we write down the Bogoliubov-de Gennes (BdG) Hamiltonian $H = \sum_k \Phi_k^* \tilde{H} \Phi_k$ for $\Phi_k = (c_k, i\sigma_y c^*_k)^T$. In the continuum limit at $\vec{P}_+$ (similar expressions are obtained for $\vec{P}_-$)

$$\tilde{H} = \begin{pmatrix} h_+(\vec{q}) & \Delta \sigma_0 \\ \Delta \sigma_0 & -h_-(\vec{q}) \end{pmatrix},$$

(9.22)

with $h_+(-\vec{q})$ defined in Eq. [9.6]. The quasiparticle spectrum corresponding to this BdG Hamiltonian is

$$E(\vec{q}) = \pm[q^2 + \Delta^2 + \mu^2 \pm 2(\Delta^2 q_x^2 + \mu^2 q_y^2)^{1/2}]^{1/2},$$

(9.23)

which has nodes at $q_x = q_y = 0$, $q_z = \pm \sqrt{\Delta^2 + \mu^2}$, both with chirality of +1. Near the nodes
\[ |q_x|, |q_y| \ll |q_z|, |\mu|, \] we obtain the anisotropic Weyl spectrum
\[ E(\vec{q}) \approx \pm \left[ (q_z \pm \sqrt{\Delta^2 + \mu^2})^2 + q_\perp^2 (1 + \frac{\mu^2}{\mu^2 + \Delta^2}) \right]^{1/2}, \] (9.24)

with \( q_\perp = (q_x, q_y) \). At zero chemical potential, this is similar to the results of Meng and Balents\[^{202}\] who considered the proximity effect of undoped Weyl semimetals. The effect of nonzero chemical potential is to simply shift the Weyl nodes located at \( q_z = \pm \Delta \) at \( \mu = 0 \), to \( q_z = \pm \sqrt{\Delta^2 + \mu^2} \).

Because of the non-trivial winding number carried by the nodes, the nodal points are robust against small perturbations. The only way to gap out the nodes is to undergo a pair-annihilation of nodes with the opposite winding numbers, and the nodal points are topologically stable as long as they are separated enough in momentum space. Strikingly, this nodal structure implies that there will be a zero-energy state on the surface which should be detectable in experiment. This is similar to \(^3\)He-A which is an odd-parity pairing state, while our superconducting phase is realized by the even-parity pairing.

### 9.3.2 \( \Gamma^1 \)-FFLO state

The singlet component of the \( \Gamma^1 \)-FFLO state is fully gapped with a mean field pair potential
\[ H_{\text{pair}}^{\text{FFLO}} = \Delta c^\dagger_\alpha (\vec{k} + \vec{P}_+)(i\sigma^y)^{\alpha\beta} c^\dagger_\beta (-\vec{k} + \vec{P}_+) \pm (\vec{P}_+ \leftrightarrow \vec{P}_-) \] (9.25)
with center-of-momentum of \( 2\vec{P}_\perp \). In the low-energy theory, it can be represented by the \textit{intra-node} pairing \( \sim \Delta \sum_{\vec{q}} \psi^\dagger_{a,\alpha}(\vec{q})(i\sigma^y)^{\alpha\beta}\psi^\dagger_{a,\beta}(-\vec{q}) \).

It is known that some two-dimensional FFLO states with strong spin-orbit coupling and parallel magnetic field are unstable against weak disorder\[^{199, 209}\]. In contrast, the FFLO state discussed in this paper is found to be robust against weak disorder. In fact, the structure of the FFLO state Eq. (9.13) and Eq. (9.25) is more similar to the even/odd-parity state of the doped topological insulators studied in reference\[^{210}\] than usual FFLO states in the two spatial dimension. This similarity is manifested if we write down the pairing for the Weyl fermions in the continuum limit in the helicity eigenstates
\[ \Delta_\pm \propto e^{i\phi} \left[ \langle \psi_+ (\vec{q}) \psi_+ (-\vec{q}) \rangle \pm \langle \psi_- (\vec{q}) \psi_- (-\vec{q}) \rangle \right], \] (9.26)
which corresponds to Eq. (5) of reference\[^{210}\]. Within this Cooper channel, we add a scalar disorder term to the Hamiltonian
\[ H_{\text{imp}} = V_{\text{imp}} \sum_{\vec{k}, \vec{p} \in \text{FS}} c^\dagger_{k,\sigma} c_{p,\sigma} \sum_{\vec{q}, \vec{l} \in \text{FS}} V_{ab}^{\vec{q},\vec{l}} \psi^\dagger_{a,\vec{q}} \psi_{b,\vec{l}} \] (9.27)
The matrix element \( V_{ab}^{\vec{q},\vec{l}} \) is given by
\[ V_{ab}^{\vec{q},\vec{l}} = V_{\text{imp}} \left( \frac{\langle \vec{q} | \vec{l} \rangle}{\langle \vec{q} | \vec{l} \rangle} \right), \] (9.28)
where we have used the standard normalized spin state \( \hat{q} \cdot \vec{\sigma} |\hat{q}\rangle = |\hat{q}\rangle \) and \( \bar{q} \cdot \vec{\sigma} |\bar{q}\rangle = |\bar{q}\rangle \) with \( \hat{q} = \frac{q}{|q|} \) and \( \bar{q} = (q_{\perp}, -q_z)/|q| \). With this impurity scattering, the self-energy can be worked out in the self-consistent Born approximation, and we find that the correction to the self-energy and the Cooperon diagram due to disorder are exactly of the same form as obtained by Michaeli and Fu[210]. In fact, the only difference between the FFLO state \( \Delta_{\pm} \) in Eq. (9.25) and the even/odd-parity paired states of reference[210] is phase factors in the matrix elements of \( V_{\vec{k},\vec{l}}^{ab} \) in Eq. (9.28) which does not show up in the corrections to the self-energy, the Cooperon diagram, and the pairing susceptibilities. Thus we conclude that the critical temperature of \( \Gamma^1 \)-FFLO states is not affected by the disorder and thus \( \Gamma^1 \)-FFLO state is robust.

### 9.4 Conclusion

In conclusion, we have studied the possible superconducting states of doped inversion-symmetric Weyl semimetals. We considered a concrete lattice model realizing a Weyl semimetal and found that the FFLO state has a lower energy than the even-parity state if the interaction is phonon-mediated, and the phase is argued to be stable against disorder. Though the even-parity state is less favored in energy than the FFLO state, it interestingly provides an electronic analogue of \( ^3\)He-A phase.

We remark briefly on the implication of our work for superconducting states of Weyl semimetal models other than the one studied in this paper. Among the many proposals for the Weyl semimetal phase, we restrict ourselves to the models based on the topological insulators[26, 27] with the time-reversal breaking perturbation.

\[
H = v\tau^y \vec{\sigma} \cdot \vec{k}_{\perp} + \tau^x k_z + m\sigma^z \tag{9.29}
\]

The typical symmetry of the model is \( I \times C_n (\times M, \text{Mirror symmetry}) \) where \( I \) is the inversion symmetry and \( C_n \) is the \( n \)-fold lattice rotation symmetry along a certain axis (for the model based on Bi\(_2\)Se\(_3\)[27], we have \( n = 3 \)). Due to the strong spin-orbit interaction, the spatial symmetry operation involves the spin/orbital operations, e.g., \( I : \vec{k} \rightarrow -\vec{k} \) should involve \( \tau^y \), and \( \tau^y H(-\vec{k}) \tau^y = H(\vec{k}) \) (the lattice rotation will involve a spin rotation). Note that these symmetry considerations already manifest the similarity between the realistic model and the simplified model Eq. (9.2), and this similarity becomes much clearer if we go to the low-energy theory of Eq. (9.29). It is not difficult to confirm that the low-energy theory is identical to Eq. (9.6), and hence we will have similar superconducting states, FFLO and electronic analogues of \( ^3\)He-A, in the more realistic model. Hence, we predict that the superconducting states we found should show up in other proposals for Weyl semimetals.

Note that FFLO state Eq. (9.25) shows a density modulation pinned by the momentum of the Weyl nodes (which is reminiscent of the field-induced charge density wave[24] of the Weyl semimetals). Many experimentally available Weyl semimetals have a large number of Weyl nodes, for example the irridates which have 24 nodes[23] (or an inversion-symmetry broken
Weyl semimetal has at least four Weyl nodes\(^{196}\)). While our minimal model calculation here does not guarantee that the FFLO state will be the lowest energy state in such systems, at minimum it suggests that it will be a competing state. In this case the FFLO state can have multiple centers of momenta. This directly implies that there will be interesting density modulation patterns which are fully determined by the position of the Weyl nodes. (This is true at least at the level of mean field theory which ignores the effect of \(O(\Delta^4)\) terms in the Landau-Ginzburg theory. \(O(\Delta^4)\) terms can potentially melt this pattern).

We also note that FFLO state can host interesting half-quantum vorticies discussed in reference\(^{211}\). In the FFLO state, we have two independent superconducting order parameters \(\Delta(\pm \vec{P}) \propto \exp(\pm 2i\vec{P} \cdot \vec{r})\), i.e., the order parameter space is \(S^1 \times S^1\). The half-quantum vortex corresponds to a unit “winding” of the phase of the \(\Delta(\vec{P})\) while the phase of the \(\Delta(-\vec{P})\) does not wind. On the other hand, the Fermi surface around the Weyl node at \(\vec{P}\) encloses the \(\pi\)-Berry phase\(^{212}\) which signals that there will be a gapless “chiral” Majorana mode at the core of the half-quantum vortex. Furthermore, this implies that a full quantum vortex will be a composite of the two half-quantum vortices and each half-quantum vortex will have a chiral mode. Thus the full quantum vortex will host a helical Majorana mode. In contrast to the related case\(^{212}\), this helical Majorana mode is not symmetry protected and is therefore generally gapped out. Furthermore, the helical Majorana mode can be understood as the critical point between a weak pairing state and a strong pairing state in a 1D p-wave superconductor\(^{115}\). There are two possible phases for the full quantum vortex depending on the sign of “mass gap” for the helical mode\(^{115}\) and in a nontrivial phase there will be a Majorana fermion at the end of the vortex.

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Bibliography


Part IV

Appendix
Chapter 10

Appendix: crystal momenta of $BF$ theory

We list the crystal momenta of each theory (we denote “e×e lattice” as even-by-even lattice, and “e×o lattice” as even-by-odd lattices, etc)

(1) $\{(I, 0), (I, 0)\}$ is [0000] Z2 spin liquid
(2) $\{(I, u_x), (I, 0)\}$
   e×e lattice: $(\pi, 0), (\pi, 0), (0, 0), (0, 0)$
   e×o lattice: $(\pi, 0), (\pi, 0), (0, 0), (0, 0)$
   o×e lattice: $(\pi, 0), (\pi, 0), (0, 0), (0, 0)$
   o×o lattice: $(\pi, 0), (\pi, 0), (0, 0), (0, 0)$
(3) $\{(I, 0), (I, u_y)\}$
   e×e lattice: $(0, \pi), (0, \pi), (0, 0), (0, 0)$
   e×o lattice: $(0, \pi), (0, \pi), (0, 0), (0, 0)$
   o×e lattice: $(0, \pi), (0, \pi), (0, 0), (0, 0)$
   o×o lattice: $(0, \pi), (0, \pi), (0, 0), (0, 0)$
(4) $\{(I, u_x), (I, u_y)\}$ is [1111] Z2 spin liquid
(5) $\{(O^t, 0), (O^t, 0)\}$ is [0110], [1001] Z2 spin liquid
(6) $\{(O^t, u_x), (O^t, 0)\}$ $([t_x, t_y] \neq 0)$
(7) $\{(O^t, 0), (O^t, u_y)\}$ $([t_x, t_y] \neq 0)$
(8) $\{(O^t, u_x), (O^t, u_y)\}$
   e×e lattice: $(\pi, \pi), (\pi, 0), (0, 0), (0, 0)$
   e×o lattice: $(0, 0), (0, 0)$
   o×e lattice: $(0, 0), (0, 0)$
   o×o lattice: $(0, 0), (0, 0)$
(9) $\{(O^t, 0), (I, 0)\}$ is [0101], [1010] Z2 spin liquid
(10) $\{(O^t, 0), (I, u_y)\}$ $([t_x, t_y] \neq 0)$
(11) $\{(O^t, u_x), (I, 0)\}$
   e×e lattice: $(\pi, 0), (\pi, 0), (0, 0), (0, 0)$
e\times o lattice: (\pi,0),(\pi,0),(0,0)(0,0)
o\times e lattice: (0,0),(0,0)
o\times o lattice: (0,0),(0,0)

(12) \{\{O^t, u_x\},\{I, u_y\}\} ([t_x, t_y] \neq 0)
(13) \{\{I, 0\},\{O^t, 0\}\} is [1100],[0011] Z2 spin liquid
(14) \{\{I, u_x\},\{O^t, 0\}\} ([t_x, t_y] \neq 0)
(15) \{\{I, 0\},\{O^t, u_y\}\} 
   e\times e lattice: (0, \pi),(0, \pi),(0,0),(0,0)
   e\times o lattice: (0,0),(0,0)
   o\times e lattice: (0, \pi),(0, \pi),(0,0),(0,0)
   o\times o lattice: (0,0),(0,0)
(16) \{\{I, u_x\},\{O^t, u_y\}\} ([t_x, t_y] \neq 0)

We looked at the patterns of the crystal momenta of the Z2 spin liquids\[98] and found four Z2 indices of Z2 spin liquids which match these patterns. Note that the classes (5) – (16) of BF theories have the gapless edge state.
Chapter 11

Appendix: helical state at domain wall

We show that if the exciton mass has a “real” domain wall (i.e., passes through zero with some fixed phase), there is a topological helical state. Without loss of generality, let the exciton mass $\Delta(y) \to \Delta_0 > 0$ for $y \to -\infty$, and $\Delta \to -\Delta_0 < 0$ for $y \to \infty$ with $\Delta(y) \to 0$ as $y \to 0$. Then we have a helical edge state localized at $y = 0$. In terms of the four-spinor, the helical states are $\Psi_+(k) \sim \exp(ikx) \exp(-\int_0^y \Delta(y)dy)|1, 1, 1, -1\rangle^T$ with $E(k) = k$ and $\Psi_-(k) \sim \exp(ikx) \exp(-\int_0^y \Delta(y)dy)|1, -1, 1, 1\rangle^T$ with $E(k) = -k$ and two fermionic states $\Psi_+(k)$ and $\Psi_-(k)$ are the Kramer pair. These 1D state is protected when $T$-symmetry at the domain wall is conserved as for spin Hall edge states. Thus, this helical state localized at the domain wall reflects the underlying topological states. This spin Hall type physics can be best understood if we look at the matrix form of the Hamiltonian $H = \Psi^\dagger H \Psi$ with the proper unitary transformation from the original bases,

$$H = \begin{bmatrix} \Delta & p_+ & 0 & 0 \\ p_- & -\Delta & 0 & 0 \\ 0 & 0 & -\Delta & p_+ \\ 0 & 0 & p_- & \Delta \end{bmatrix} \quad (11.1)$$

As the helical 1D metal is protected only if $T$-symmetry is conserved at the domain wall, we set $m = 0$ near the domain wall. Now, it is clear that when $\Delta$ has the domain wall at $y = 0$, the upper two spinor has the chiral mode propagating in the positive $x$, and the lower two spinor has the chiral mode propagating in the negative $x$. Further consideration shows that two modes are a Kramer pair and are protected from generating a gap only when $T$-symmetry is conserved. Note that a general domain wall where the phase difference in the (generally complex) exciton mass is not $\pi$ need not have this bound state.
Chapter 12

Appendix for chapter 9

12.1 Appendix: continuum Weyl fermions: interaction, and gap equation

In this appendix, we derive the equations related to the continuum theory from the microscopic lattice model Eq. (9.2). First of all, let us derive the interaction Eq. (9.9) for the Weyl fermions. The interaction (9.3) in the momentum space is

\[ H = \sum_{\vec{k},\vec{p},\vec{q}} V_{\vec{k}} c_{\vec{p},\sigma}^\dagger (\vec{q} - \vec{k}) c_{\vec{q},\tau}^\dagger c_{\vec{q},\sigma} (\vec{p}), \]

(12.1)

with \( V_{\vec{k}} = V_0 + V_1 (\cos(k_x) + \cos(k_y) + \cos(k_z)) \). For the BCS pairings where the center of momentum is at zero \( \vec{q} = -\vec{p} \), we obtain the pairing potential

\[ H = \sum_{\vec{p},\vec{q}} V_{\vec{p} - \vec{q}} c_{\vec{p},\sigma}^\dagger c_{\vec{q},\tau}^\dagger c_{\vec{q},\sigma} (\vec{p}). \]

(12.2)

As the electron operators that we are concerning are localized near the Weyl points, we expand the electron operators near the Weyl points. This can be easily done by plugging \( \vec{p} = \vec{k} \pm \vec{P} \) and \( \vec{q} = \vec{l} \pm \vec{P} \) with \( \vec{P} = (0, 0, Q) \) into Eq. (12.2). For example, the interaction (12.2) includes the interaction

\[ \sim V_{(\vec{k}+\vec{P})-(\vec{l}+\vec{P})} \psi_{+\tau,\sigma}^\dagger (\vec{k}) \psi_{-\tau,\sigma}^\dagger (-\vec{k}) \psi_{-\tau,\sigma} (-\vec{l}) \psi_{+\tau,\sigma} (\vec{l}), \]

(12.3)

which allows us to identify \( V_{+(+-)} (\vec{k}-\vec{l}) = V_{(\vec{k}+\vec{P})-(\vec{l}+\vec{P})} \). Similarly, we can identify \( V_{-(++)} (\vec{k}-\vec{l}) = V_{(\vec{k}-\vec{P})-(\vec{l}-\vec{P})} \), \( V_{+(--)} (\vec{k}-\vec{l}) = V_{(\vec{k}+\vec{P})-(\vec{l}+\vec{P})} \), and \( V_{(+-)} (\vec{k}-\vec{l}) = V_{(\vec{k}+\vec{P})-(\vec{l}-\vec{P})} \). After
this identification, it is straightforward to expand for the small \( \vec{k}, \vec{l} \) to obtain
\[
V^{-+;+-} = V^{+-;--} = V_0 + 3V_1 - \frac{V_1}{2}(\vec{k} - \vec{l})^2,
\]
\[
V^{-+;+-} = V_0 + 2V_1 + V_\perp + V^+, \\
V^{+-;--} = V_0 + 2V_1 + V_\perp + V^-, \\
V_\perp = -\frac{V_1}{2}(\vec{k}_\perp - \vec{l}_\perp)^2,
\]
\[
V^+_\perp = V_1\cos(2Q)(1 - \frac{1}{2}(k_z - l_z)^2) + (k_z - l_z)\sin(2Q)), \\
V^-_\perp = V_1\cos(2Q)(1 - \frac{1}{2}(k_z - l_z)^2) - (k_z - l_z)\sin(2Q)).
\] (12.4)

Next, we discuss the mean field pairing terms in the continuum theory derived from the lattice model. The possible pairing states from the interaction Eq. (9.3) are listed in the table 9.1. The typical form of the pairing term can be represented by
\[
H_{\text{pair}} = \sum \Delta^{\sigma \tau}_c(\vec{k})\Gamma^{\sigma \tau}_c(\vec{k})^{\dagger} \psi^{\dagger}_{\tau,\sigma}(\vec{k}) \langle \psi_{\sigma,\tau}(-\vec{k}) \rangle.
\] (12.5)

As we now have the explicit form of the pairing term and the interaction for the Weyl fermions, it is now straightforward to obtain the gap equation for each ansatz by solving
\[
\Delta_{\sigma \tau}(\vec{k}) = \Delta(\Gamma^{\sigma \tau}_c(\vec{k})).
\] (12.7)

As we now have the explicit form of the pairing term and the interaction for the Weyl fermions, it is now straightforward to obtain the gap equation for each ansatz by solving
\[
\Delta_{\sigma \tau}^{ab}(\vec{p}) = \sum \chi^{\sigma \tau}_c(\vec{k})^{\dagger} \Gamma^{\sigma \tau}_c(\vec{k}) \langle \psi_{\tau,\sigma}(\vec{k}) \rangle.
\] (12.8)

For example, the gap equation for the singlet pairing component \( \Delta_{\sigma \tau}^{ab} = \Delta(\Gamma^{1}_{c\sigma \tau}(\vec{k})) \) in Eq. (12.6) is
\[
\Delta = \frac{1}{4} \sum \chi^{\sigma \tau}_c(\vec{k})^{\dagger} V^{abcd}(\vec{p} - \vec{k}) \langle \psi_{\tau,\sigma}(\vec{k}) \rangle.
\] (12.9)

The similar expressions of the gap equations hold for other pairings and the results are following. For the triplet pairing component in \( \Gamma^{1} (C_4 = 1) \), there are two pairing channels
$\sim \Delta_I(X - iY)(\sigma^x + i\sigma^y)(i\sigma^y) + \Delta_{II}(X + iY)(\sigma^x - i\sigma^y)(i\sigma^y)$ which can mix each other (see table 9.1)

$$\Delta_I = \frac{1}{8} \sum_{\vec{k}} \left\{ [V^{x,y,cd}(\vec{k}) - iV^{y,y,cd}(\vec{k})] [X_{cd}(\vec{k}) + iY_{cd}(\vec{k})] \right\},$$

$$\Delta_{II} = \frac{1}{8} \sum_{\vec{k}} \left\{ [V^{x,y,cd}(\vec{k}) + iV^{y,y,cd}(\vec{k})] [X_{cd}(\vec{k}) - iY_{cd}(\vec{k})] \right\}, \quad (12.9)$$

where we define the following compact notations

$$V^{x,cd}(\vec{k}) = \frac{\sum_{\vec{p} \in d\Omega} (\tau^x)_{ab} P_x V^{ab,cd}(\vec{k} - \vec{p})}{\sum_{\vec{p} \in d\Omega} P_x^2}$$

$$V^{y,cd}(\vec{k}) = \frac{\sum_{\vec{p} \in d\Omega} (\tau^x)_{ab} P_y V^{ab,cd}(\vec{k} - \vec{p})}{\sum_{\vec{p} \in d\Omega} P_y^2} \quad (12.10)$$

where $d\Omega$ is the thin shell around the Fermi surface. The width of the shell is determined by the phenomenological parameter (Debye frequency) defining the electron-phonon coupling, e.g., $t \times d\Omega$ is the characteristic energy of the phonons.

$$X_{cd}(\vec{k}) = \langle \psi_{c,\beta}(-\vec{k}) | -i\sigma^y \sigma^x \rangle_{\beta}^\alpha \langle \psi_{d,\alpha}(\vec{k}) \rangle$$

$$Y_{cd}(\vec{k}) = \langle \psi_{c,\beta}(-\vec{k}) | -i\sigma^y \sigma^y \rangle_{\beta}^\alpha \langle \psi_{d,\alpha}(\vec{k}) \rangle$$

$$Z_{cd}(\vec{k}) = \langle \psi_{c,\beta}(-\vec{k}) | -i\sigma^y \sigma^z \rangle_{\beta}^\alpha \langle \psi_{d,\alpha}(\vec{k}) \rangle \quad (12.11)$$

with the expectation value taken for the mean field superconducting state.

For $\Gamma^2$ pairing ($C_4 = -1$), there are two pairing channels $\sim \Delta_I(X + iY)(\sigma^x + i\sigma^y)(i\sigma^y) + \Delta_{II}(X - iY)(\sigma^x - i\sigma^y)(i\sigma^y)$ which can mix each other (see table 9.1), and the self-consistency requires

$$\Delta_I = \frac{1}{8} \sum_{\vec{k}} \left\{ [V^{x,y,cd}(\vec{k}) - iV^{y,y,cd}(\vec{k})] [X_{cd}(\vec{k}) + iY_{cd}(\vec{k})] \right\},$$

$$\Delta_{II} = \frac{1}{8} \sum_{\vec{k}} \left\{ [V^{x,y,cd}(\vec{k}) + iV^{y,y,cd}(\vec{k})] [X_{cd}(\vec{k}) - iY_{cd}(\vec{k})] \right\}, \quad (12.12)$$

For $\Gamma^3, \pm$ pairing ($I = -1$ and $C_4 = \pm i$), the analogous expressions can be derived by similar methods.

### 12.2 Appendix: FFLO state on surface of TIs

In this appendix, we will propose a possible FFLO state from the surface state of the strong topological insulator under the parallel magnetic field. As far as the magnetic field is
Table 12.1: Symmetry classification of distinct BCS pairing order parameters in (12.18), corresponding to different odd-parity irreducible representations (IRRs) of point group $C_4$. Here $(X, Y, Z)$ are basis functions for the momentum-space pairing function $\Delta(\mathbf{k})$, denoting e.g. the function $(\sin(p_x), \sin(p_y), \sin(p_z))$ or other functions with the same symmetry.

<table>
<thead>
<tr>
<th>IRR</th>
<th>$C_4$</th>
<th>basis functions of $\Delta(\mathbf{k})$</th>
<th>Nodes?</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_u$</td>
<td>1</td>
<td>$Z$</td>
<td>N/A</td>
</tr>
<tr>
<td>$B_u$</td>
<td>$-1$</td>
<td>$XYZ$ or $(X^2 - Y^2)Z$</td>
<td>line nodes</td>
</tr>
<tr>
<td>$E_{u+}$</td>
<td>$i$</td>
<td>$X + iY$</td>
<td>N/A</td>
</tr>
<tr>
<td>$E_{u-}$</td>
<td>$-i$</td>
<td>$X - iY$</td>
<td>N/A</td>
</tr>
</tbody>
</table>

In-plane, the only coupling from the magnetic field to the surface state is Zeeman coupling. Then, the Zeeman coupling will shift the Fermi surface uniformly along the direction to the magnetic field. The low-energy theory is

$$H = v\sigma \cdot (\mathbf{k} + g\mathbf{B}/v) - \mu.$$ \hspace{1cm} (12.13)

If there is a phonon-mediated $surface$ transition toward superconducting state, the superconducting state should be at the finite center-of-momentum pairing. We model the phonon-mediated attractive interaction as

$$\delta H = U \sum_{\mathbf{k}} n_{\mathbf{k}} n_{-\mathbf{k}},$$ \hspace{1cm} (12.14)

which is local in the real space and uniform in the momentum space. This implies that the pairing will be uniform in the momentum space, hence we can single out a single pairing state $\Delta(\mathbf{r}) \propto \exp(-2i\mathbf{Q} \cdot \mathbf{r})$ with $\mathbf{Q} = g\mathbf{B}/v$,

$$H_{\text{pair}} = \Delta(\mathbf{Q}) c_{\alpha}^{\dagger}(\mathbf{Q} + \mathbf{k})(i\sigma^y)^{\alpha\beta} c_{\beta}^{\dagger}(\mathbf{Q} - \mathbf{k}) + h.c.$$ \hspace{1cm} (12.15)

Hence, we have shown that FFLO state can show up, at least in the mean field theory, in the surface state of strong topological insulators under the in-plane magnetic field. What would be the effect of weak disorder to this phase? By following the discussion in reference [209], we conclude that this FFLO state should be robust against the weak neutral disorder (this problem corresponds to the problem where the disorder scatters electrons only within the $single$ Rashba band in the reference).

### 12.3 Appendix: symmetry classification of pairing order parameters in two-band model

In this section we classify possible BCS-type pairing order parameters in two-band model (9.2) with interactions, as long as interaction terms do not break the point group symmetry...
of tight-binding model \([9.2]\). These different pairing order parameters are characterized by distinct irreducible representations of group \(C_4\) generated by 90 degree rotation along \(\hat{z}\)-axis.

When the Weyl semimetal described by two-band model \([9.2]\) is doped slightly with \(\mu > 0\) and \(|\mu/t| \ll 1\), the Fermi surface consists two electron pockets around Weyl nodes \(\pm \vec{P} = (0, 0, \pm Q)\). The tight-binding model \([9.2]\) can be diagonalized into \(H(\vec{k}) = \vec{d}_{\vec{k}} \cdot \vec{\sigma} - \mu = U_{\vec{k}}^\dagger (\varepsilon_{\vec{k}} \sigma^z - \mu) U_{\vec{k}}\), where \(U_{\vec{k}} = \begin{pmatrix} u_{\vec{k}} & v_{\vec{k}} \\ -v_{\vec{k}}^* & u_{\vec{k}}^* \end{pmatrix}\) is a 2 \(\times\) 2 unitary matrix. Hence the low-energy degree of freedoms on the Fermi surface \(\varepsilon_{\vec{k}} = \mu\) are

\[
\vec{f}_{\vec{k}} = u_{\vec{k}} c_{\vec{k}, \uparrow} + v_{\vec{k}} c_{\vec{k}, \downarrow},
\]  

and according to inversion symmetry we have \(U_{-\vec{k}} = U_{\vec{k}} \sigma_z\) and

\[
\vec{f}_{-\vec{k}} = u_{\vec{k}} c_{-\vec{k}, \uparrow} - v_{\vec{k}} c_{-\vec{k}, \downarrow}.
\]

For a general electronic model with \(C_{4h}\) symmetry (but no time reversal), the Fermi surface is nondegenerate. Therefore a generic BCS-type pairing term is written as

\[
H_{\text{pair}} = \sum_{\vec{k}} \left( \Delta(\vec{k}) \vec{f}_{\vec{k}}^\dagger \vec{f}_{-\vec{k}}^\dagger + \text{h.c.} \right),
\]  

Apparently the pairing order parameter \(\Delta(-\vec{k}) = -\Delta(\vec{k})\) is a odd-parity function (instead of a 2 \(\times\) 2 matrix). One can always choose a gauge so that under \(C_4\) symmetry in \([9.4]\):

\[
C_4 : \quad (k_x, k_y, k_z) \rightarrow (k_y, -k_x, k_z)
\]  

the eigenvector \((u_{\vec{k}}, v_{\vec{k}})\) transforms as

\[
u_{C_4 \vec{k}} = u_{\vec{k}}, \quad v_{C_4 \vec{k}} = i \cdot v_{\vec{k}}.
\]  

In this specific gauge the operator \(f_{\vec{k}}\) transforms trivially under rotation \(C_4\) and inversion \(I\), hence the order parameter \(\Delta(\vec{k})\) should form a one-dimensional odd-parity (irreducible) representation of the symmetry group \(C_{4h}\). All possible different order parameters are classified by their symmetry and listed in Table \([12.1]\). The \(B_u\) state has nodal lines along which there are gapless excitations, while the other three BCS paired states are fully gapped.

The symmetry classification of BCS pairing order parameters are generally true for any system with \(C_{4h}\) symmetry but no time reversal (so that the Fermi surface is nondegenerate). In the specific two-band model \([9.2]\), we can relate the low-energy eigenband operators \(f_{\vec{k}}\) to original electron operators \(c_{\vec{k}, \sigma}\) through \([12.16]\), and the distinct pairing functions in the original electron basis are summarized in Table \([9.1]\).