ELECTRIC MULTIPOLe MOMENTS
AND HIGHER-ORDER TOPOLOGICAL PHASES
IN CRYSTALLINE INSULATORS AND SUPERCONDUCTORS

BY

WLADIMIR A. BENALCAZAR

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Doctoral Committee:

Professor Smitha Vishveshwara, Chair
Professor Taylor L. Hughes, Director of Research
Professor Bryce Gadway
Professor Virginia Lorenz
Abstract

This dissertation discusses extensions of the theory of polarization in crystalline insulators. The notion that electronic wave functions of energy bands in crystalline insulators have Berry phases associated with the positions of electronic charge is at the basis of our understanding of topological band theory. We show, by using the Berry phase formulation and generalizations of it, as well as by exact diagonalization of tight-binding models, that crystalline insulators can generate charge and polarization patterns compatible with the notion of quadrupole and octupole electric moments. In the presence of certain symmetries, these moments are quantized, and their boundary signatures fractionalized. These higher multipole moments then correspond to new symmetry-protected topological phases (SPTs). A salient signature of these SPTs is the existence of zero-dimensional, corner-localized mid-gap energy states. We then study topological crystalline superconductors, in which these zero-dimensional mid-gap states amount to the existence of Majorana bound states (MBS). We thoroughly classify these systems when rotational group symmetries are enforced, and investigate the existence of zero-dimensional MBS trapped at topological defects in these crystals. The finding of these higher multipole moments or generalizations of them to other platforms constitute a new paradigm for the realization of symmetry protected topological phases.
To my mother
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Chapter 1

Introduction

1.1 Background

At the beginning of last century, x-ray crystallography confirmed the periodic structure of crystals. Setting defects aside, an ideal crystal consists of identical building blocks - atoms or groups of atoms - that repeat periodically. This discovery crucially helped in the understanding of macroscopic properties of a wide range of materials. By studying vibrations in atomic lattices, a picture of a crystal as a gas of phonons emerged which explained the heat capacity and thermal conductivity in crystals.

A similar picture was initially expected to follow for the electrons in a crystal. The valence electrons of the individual atoms that make the lattice are donated to the entire crystal, effectively constituting a gas of free electrons, but with a crucial difference, first postulated by Fermi: a gas of electrons had to be subjected to the Pauli exclusion principle. The Fermi free electron theory was successful not only in describing properties derived from the kinetic characteristics of the conduction electrons in metals but also gave the correct expressions for the electronic contribution to the heat capacity. It was, however, incapable of describing the strikingly different behaviors between metals and insulators.

The solution to this problem came from Bloch, who extended the Fermi free electron theory to include the periodicity of the potential that arises from the atomic lattice. Specifically, he found that the solution to the Schrödinger equation for a particle in periodic potential $V(r)$, i.e. one which obeys $V(r) = V(r + a)$ for some lattice constant $a$, takes the form

$$\psi_k(r) = e^{ik \cdot r} u_k(r), \quad (1.1)$$

where $u_k(r)$ is a function that is periodic with the same periodicity of the lattice, $u_k(r) = u_k(r + a)$. The plane waves of free electrons are thus modified only by a periodic modulation [1]. This consideration, however, was crucial, as it leads to the emergence of the bandgap. The dispersion curves of electrons in crystals are not continuous; they have gaps, forbidden regions of energy over which no electrons can be found.
at any crystal momentum $k$. These gaps, arising from the interaction of the electrons with the lattice, thus separate well-defined energy bands, the filling of which determine its electronic properties; for example, a metal has partially filled bands, whereas an insulator will have bands that are either completely filled or empty.

Just as the theory of energy bands in crystals was developed along with quantum mechanics, many other developments around quantum theory explained and predicted the existence of a vast number of phenomena in condensed matter systems, including superconductivity, Bose-Einstein condensation, charge density waves, ferromagnetism, and antiferromagnetism, to name a few.

In this dissertation, our starting point is the study of crystalline insulators, from which we will then expand into other phenomena. Specifically, we will attempt to extend the theory of charge polarization to include higher electric multipole moments. The problem of calculating the charge polarization in crystalline insulators has been an outstanding problem that remained elusive for more than half a century after the development of the band theory of crystals. The difficulty stemmed from the fact that the macroscopic electric polarization of a periodic crystal cannot be unambiguously defined as the dipole of a unit cell [2] and, therefore, the absolute macroscopic polarization of a crystalline insulator is ill-defined.

The right approach to address the problem of charge polarization was laid out by a series of seminal papers in the 1980’s. In 1984, Berry showed that a quantum mechanical particle, when dragged slowly around a closed circuit, acquires a phase factor [3]. Five years later, a remarkable application of the Berry phase was put forward by Zak. Namely, in periodic solids, the Brillouin zone has a torus topology, and hence a Berry phase can be generated when the electronic wavefunctions in a crystal are ‘transported’ in the crystal momentum space $k$. Surprisingly, this Berry phase has a physical consequence: it reveals the positions of the electrons in insulating crystals [4]. In a parallel development, following the explanation of the quantization of the Hall conductance in two-dimensional insulators [5, 6], Thouless showed in 1983 that in one-dimensional periodic Hamiltonians, closed adiabatic cycles could quantize electron transport [7]. The final piece in this puzzle was put by Resta, Vanderbilt, and collaborators, when they recognized that only derivatives of the polarization -and not the polarization itself - are well-defined observables susceptible of being measured in experiments [2], essentially linking the formulation of Thouless with that of Zak, in what is now known as the modern theory of polarization in crystalline insulators [8, 9, 10, 11, 12]. This theory is formulated in terms of Berry phases, which account for the dipole moment densities in the bulk of a material, and it has its minimal realization in one dimension [13, 14] (1D). A bulk dipole moment manifests itself through the existence of boundary charges [9]. When the dipole moment densities vary over time, e.g., by an adiabatic evolution of an insulating Hamiltonian over time, electronic currents appear across the
bulk of the material where the polarization is changing [8, 9]. In particular, if adiabatic evolutions of the Hamiltonian are carried over closed cycles, the electronic transport is quantized [7]. This quantization is given by a Chern number, and, mathematically, in systems with charge conservation, is closely related to the Hall conductance of a Chern insulator [6].

A remarkable pattern develops in the topological objects describing these systems that follow a hierarchical mathematical structure as the dimensionality of space increases. For example, the expressions for the polarization $P_1$ [4, 8], the Hall conductance $\sigma_{xy}$ of a Chern insulator [5, 6, 15], and the magneto-electric polarizability $P_3$ of a three-dimensional (3D) time-reversal invariant or inversion symmetric topological insulator [16, 17, 18, 19], are given by

$$P_1 = -\frac{e}{2\pi} \int_{BZ} \text{Tr} [A] \quad (1.2)$$

$$\sigma_{xy} = -\frac{e^2}{2\pi\hbar} \int_{BZ} \text{Tr} [dA + iA \wedge A] \quad (1.3)$$

$$P_3 = -\frac{e^2}{4\pi\hbar} \int_{BZ} \text{Tr} \left[ A \wedge dA + \frac{2i}{3} A \wedge A \wedge A \right], \quad (1.4)$$

where $BZ$ is the Brillouin zone in one, two, and three spatial dimensions respectively, and $A$ is the Berry connection, with components $[A_i(k)]^{mn} = -i\langle u^m_k | \partial_k | u^n_k \rangle$, where $| u^n_k \rangle$ is the Bloch function of band $n$, and $m, n$ run only over occupied energy bands.

This hierarchical mathematical structure positions the concept of charge polarization at the basis of the field of topological band theory. This theory differs from ordinary band theory in that it distinguishes different phases not by the information on the energy spectrum of a crystal, but by the topological information encoded in the energy band’s eigenstates of the crystal. The electronic eigenstates are used to construct topological invariants that characterize these phases and are tied to quantized physical observables. For example, in 1D insulators in the presence of inversion symmetry, the polarization in Eq. (1.2) is quantized to either 0 or $\frac{e}{2}$ [4, 16, 18, 19]. In principle, for every discrete symmetry, there must be phases classified by topological invariants, and which exhibit distinct physical properties.

The discovery of symmetry protected topological insulators and superconductors (SPTs) has been one of the most exciting developments in condensed matter physics in the last ten years [20, 21]. The most notable symmetry protection is due to time-reversal symmetry [22], but by now the list of possible symmetry protected topological states has vastly expanded. Fermionic SPTs with time-reversal, charge-conjugation, and/or chiral symmetries [23] in all spatial dimensions were categorized in a periodic classification table of topological insulators and superconductors [24, 16, 25]. In fact, a complete topological band theory would include topological classifications based on all point-group symmetries in addition to the discrete symmetries.
of time-reversal, charge-conjugation, and chirality. This challenge has been met through the work of several different groups which have begun classifying topological states protected by reflection [26, 27, 28, 29, 30], inversion [31, 32, 18, 19], rotation [33, 34, 35, 36, 37], non-symmorphic symmetries [38, 39, 40] and more [41, 42, 43, 44, 45, 46, 47, 48, 49, 50].

1.2 Motivation

The natural mathematical structure connecting the topological phenomena described by the invariants in Eqs. 1.2-1.4 seems to have diverted the attention from a more natural physical generalization of the dipole moment: higher multipole moments. In the classical theory of dielectrics, it is well known that the electric potential due to a charge distribution in an insulator can be accounted for as arising from contributions of different multipole moments, i.e., distributions of charge that obey certain symmetry properties. The simplest multipole is the electric monopole moment, equal to the total charge in the material, then there is the electric dipole moment [described by Eq. (1.2)], the electric quadrupole, and so on. Knowing the results for the dipole moment in crystalline insulators, some natural questions arise: can these higher moments be found in crystalline insulators? If so, what is the mathematical structure for the higher moments that is analogous to the Berry phase description of the dipole moment? Can these higher moments be quantized? In this dissertation, we will first study these questions.

Motivated by the existence of quantized higher multipole moments, we will then make connections to explore similar quantized features in other symmetry-protected topological phases. These so-called higher-order topological insulators promise to open new possibilities for the realization of quantized observables in SPT phases - one of the most fundamental and sought-after properties in condensed matter physics. In particular, we will study topological superconductors. These are radically different platforms that manifest intriguing quasiparticles known as Majorana bound states (MBS). The realization of MBS [51] has become one of the most exciting challenges in the condensed matter community [52, 20, 21, 53, 54] due to its non-Abelian fusion and braiding characteristics [55, 56] and promising prospects in topological quantum computing [57, 58, 59, 60, 61, 62].

Along with the study of these superconductors, we will attempt to gain an understanding of how these novel phases manifest at topological defects in lattices. We will study, using K-theory and simulations, under which circumstances disclinations and dislocations can trap MBS at their cores.
1.3 Contributions

The work presented in this dissertation was built from the following publications:


   In this work, we show that bulk quadrupole and octupole moments can be realized in crystalline insulators. We also devise a new paradigm based on nested Wilson loops that connect the topology of the bulk of a crystalline insulator to the topology of the effective lower dimensional Hamiltonian of its boundary.


   In this work, we extend the theory of the first publication to systematically address the problem of calculating bulk and boundary multipole moments in crystalline insulators. We also discuss adiabatic pumping phenomena associated with these higher multipole moments and predict the existence of a higher-order topological insulator, which has insulating bulk and surfaces, but chiral metallic hinges.


   In this work, we classify discrete-rotation symmetric topological crystalline superconductors in two dimensions and provide the criteria for the existence of zero-energy Majorana bound states to be present at composite topological defects made of magnetic flux, dislocations, and/or disclinations.

Additionally, the two appendices, which are complementary to the theory presented in the main text, summarize work published in the following papers:


   In this work, we build a model for a metamaterial analog of a quadrupole insulator, first proposed in Ref. [63], with arrays of microwave resonators. This study, along with a parallel development in a different platform [64], verifies the spectral properties predicted by our theory. Furthermore, this
work proves that the observed features present the robustness expected for topologically protected phenomena.


In this work, we build a hexagonal photonic crystal characterized by the presence of corner-localized mid-gap modes. The existence of these modes is shown to be related to a nontrivial topological configuration of its energy bands. Thus, we show that upon a phase transition into a topologically trivial regime, the modes disappear. We verify the existence of these modes experimentally by propagating modes into the crystal and analyzing the dynamics of the optical field.

1.4 Overview

This dissertation is divided into two parts. In the first part, corresponding to Chapter 2, we study higher electric multipole moments in crystalline insulators. We show that crystalline insulators can host higher multipole moments and that these moments can be quantized in the presence of certain point group symmetries. Appendix A complements this chapter by presenting a metamaterial realization of the lattice corresponding to the minimal quadrupole model. In addition, this chapter describes electronic pumping phenomena and higher-order topological insulators with hinge-localized chiral modes associated with these moments.

One of the main conclusions of Chapter 2 is that topological crystalline insulators may have gapped bulk and edges, but gapless features at corners. This characteristic is further explored in the second part of this dissertation, presented in Chapter 3, in which we systematically classify topological superconductors that break time-reversal symmetry to then interrogate which topological classes can trap an odd number of Majorana bound states at the core of composite topological defects. This is clearly indicated by a number of topological indices that depend on the topological invariants that classify the superconducting phases, and holonomic quantities characterizing the topological defects. Although no experimental evidence is shown for the claims in this chapter, Appendix B complements this chapter by presenting evidence of mid-gap corner-localized modes in a photonic analog of one of the topological superconductors upon which our indices are built.

Finally, we present our conclusions and outlook in Chapter 4.
Chapter 2

Electric multipole moments in crystalline insulators

2.1 Introduction

In this Chapter, we thoroughly develop the theory of quantized electromagnetic observables in topological crystalline insulators. We discuss in detail the observables of multipole moments and their relations, both in the classical continuum theory and in the quantum-mechanical crystalline theory and also discuss the extension of the theory of polarization to account for non-quantized higher multipole moments. To carry this out we systematically extend the theory of charge polarization in crystalline insulators by taking a different route than the extension suggested by the hierarchical mathematical structure evident in Eqs. (1.2)-(1.4). Our topological structure is also of hierarchical nature, but subtly involves the calculation of Berry phases of reduced sectors within the subspace of occupied energy bands. To find the relevant subspace, we resolve the energy bands into spatially separated “Wannier bands” through a Wilson-loop calculation, or, equivalently, a diagonalization of a ground state projected position operator. We call this structure “nested Wilson loops”. It goes one step beyond the previous developments in the understanding of topological insulator systems in terms of Berry phases [65, 66, 67, 68, 69]. At its core, this nested Wilson loop structure reflects the fact that even gapped edges of topological phases can signal a nontrivial bulk-boundary correspondence when the gapped edge Hamiltonian is topological itself and inherits such nontrivial topology from the bulk.

This topological structure reveals that, in addition to bulk dipole moments, crystalline insulators can realize bulk quadrupole and octupole moments, as initially shown in Ref. [63]. Furthermore, when we allow for the adiabatic deformation and evolution of Hamiltonians having non-zero quadrupole and octupole moments we find new types of quantized electronic transport and currents, extending what is already known in the case of the adiabatic charge pumping [7]. In particular, the new types of adiabatic electronic currents are localized not in the bulk, but on edges or hinges of the material. They essentially amount to pumping a dipole or quadrupole across the bulk of the material, respectively. If the adiabatic process forms a closed cycle, the transport is quantized, i.e., the amount of dipole or quadrupole being pumped is quantized. The

\footnote{This Chapter is reproduced from Wladimir A. Benalcazar, B. Andrei Bernevig, and Taylor L. Hughes, Phys. Rev. B 96, 245115 (2017). ©2017 American Physical Society. This paper is also cited as Ref. [63] in this dissertation.}
first Chern number characterizes the 1D adiabatic pumping process; this process can be connected to a Chern insulator phase in one spatial dimension higher. The dipole pumping process in the two-dimensional (2D) quadrupole system correspondingly predicts the existence of an associated three-dimensional (3D) “hinge Chern insulator” having the same topological structure as a family of 2D quadrupole Hamiltonians forming an adiabatic evolution through a ‘nontrivial’ cycle (i.e., a cycle that connects a quantized topological quadrupole insulator with a trivial insulator, while maintaining the energy gap open). This insulator has four hinge localized modes which are chiral and disperse in opposite directions at adjacent hinges. In principle, the quadrupole pumping of the 3D octupole system would predict a four-dimensional (4D) topological phase, though we will not discuss it any further here.

### 2.1.1 Outline

In Sec. 2.2 we first define electric multipole moments within the classical electromagnetic theory, characterize their boundary signatures, and establish the criteria under which these moments are well defined.

We then start the discussion of the dipole moment in crystalline insulators in one dimension (1D) in Sec. 2.3, and in two dimensions (2D) in Secs. 2.4 and 2.5. We directly calculate the position of electrons in the crystal by means of diagonalizing the position operator projected into the subspace of occupied bands. This approach provides us with eigenstates of well defined electronic position, which we then use to extend the formulation to higher multipole moments. We discuss the symmetry constraints that quantize the dipole moments and present the case of the Su-Schrieffer-Hegger (SSH) model as a primitive model for the realization of the dipole symmetry-protected topological (SPT) phase. We further use extensions of this model that break the symmetries that protect the SPT phase and thus allow an adiabatic change in polarization and the appearance of currents. We then discuss the topological invariant that characterizes the quantization of charge transport in closed adiabatic cycles.

In Sec. 2.4, we extend the 1D treatment of the problem to 2D and introduce the concept of Wannier bands, which plays a crucial role in the description of higher multipole moments. We also characterize - in terms of Wannier bands - the topology of a Chern insulator and the quantum spin Hall insulator as examples, and make connections between the topology of a Chern insulator and the quantization of particle transport of Sec. 2.3.

In Sec. 2.5, we describe the recently found phenomenon of edge-polarization [70] and its relation to corner charge. In particular, we use this as an example that allows discriminating corner charge arising from converging edge-localized dipole moments from the corner charge arising from higher multipole moments.

We then describe the existence of the first higher multipole moment, the quadrupole moment, in Sec. 2.6.
We first present the theory in terms of the diagonalization of position operators. We derive the conditions (i.e., the symmetries) under which the quadrupole moment quantizes to $\pm \frac{5}{2}$, realizing a quadrupole SPT. We then present a concrete minimal model with quadrupole moment. We describe the observables associated with it: the existence of edge polarization and corner charge, as well as the different symmetry-protected phases associated with this model and the nature of its phase transitions. We then break the symmetries that protect the SPT to cause adiabatic transport of charge, but in a pattern that amounts to a net pumping of dipole moment. This dipole moment transport can also be quantized in an analogous manner to the charge transport in a varying dipole. We describe the invariant associated with this quantization and the extension of this principle to the creation of unusual insulators which present chiral hinge-localized dispersive modes due to its nontrivial topology.

In Sec. 2.7 we describe the existence of octupole moments. We describe the hierarchical topological structure that gives rise to higher multipole moments, as well as the minimal model that realizes a quantized octupole SPT. We also describe, by means of a concrete example, how the quantization of quadrupole transport can be realized.

### 2.2 The multipole expansion in the continuum electromagnetic theory

Since the classical theory of multipole moments, even in the absence of a lattice, has various subtleties, we will spend time reviewing it in this section. Our goal is to provide precise definitions for the dipole, quadrupole, and octupole moments in insulators as well as to extract their macroscopically observable signatures.

#### 2.2.1 Definitions

In this section, we define multipole electric moments in macroscopic materials based on classical charge configurations in the absence of a lattice. We define a macroscopic material as one which can be divided into small volume elements (voxels), as shown in Fig. 2.1, over which multipole moment densities can be defined, and in such a way that these densities can be treated as continuous functions of the position at larger length scales.

For a material divided into such voxels, the expression for the electric potential at position $\vec{r}$ due to a
Figure 2.1: Macroscopic material divided in small voxels over which the multipole moment densities are calculated. Each voxel is labeled by its center point $\vec{R}$. $\vec{r}$ is the position (far) outside the material at which the potential is calculated.

Charge distribution over space is

$$\phi(\vec{r}) = \frac{1}{4\pi\epsilon} \sum_{\vec{R}} \int_{v(\vec{R})} d^3\vec{r}' \frac{\rho(\vec{r}' + \vec{R})}{|\vec{r}' - \vec{R} - \vec{r}|},$$  \hspace{1cm} (2.1)$$

where $\rho(\vec{r})$ is the volume charge density, $\epsilon$ is the dielectric constant, $\vec{R}$ labels the voxel, and in the integral $\vec{r}'$ runs through the volume $v(\vec{R})$ of voxel $\vec{R}$. Since the voxels are much smaller than the overall size of the material, we have that $|\vec{r}'| \ll |\vec{r} - \vec{R}|$ as long as $\vec{r}$ is outside of the material and sufficiently away from it.

Then, one can expand the potential (2.1) in powers of $1/|\vec{r} - \vec{R}|$ to define the multipole moment densities

$$\rho(\vec{R}) = \frac{1}{v(\vec{R})} \int_{v(\vec{R})} d^3\vec{r}' \rho(\vec{r}' + \vec{R}) \hspace{1cm}$$

$$p_i(\vec{R}) = \frac{1}{v(\vec{R})} \int_{v(\vec{R})} d^3\vec{r}' \rho(\vec{r}' + \vec{R}) r'_i \hspace{1cm}$$

$$q_{ij}(\vec{R}) = \frac{1}{v(\vec{R})} \int_{v(\vec{R})} d^3\vec{r}' \rho(\vec{r}' + \vec{R}) r'_i r'_j \hspace{1cm}$$

$$o_{ijk}(\vec{R}) = \frac{1}{v(\vec{R})} \int_{v(\vec{R})} d^3\vec{r}' \rho(\vec{r}' + \vec{R}) r'_i r'_j r'_k \hspace{1cm} (2.2)$$

which allow to write the terms in the expansion of the potential

$$\phi(\vec{r}) = \sum_{l=0}^{\infty} \phi^l(\vec{r}),$$  \hspace{1cm} (2.3)
as

\[
\phi^0(\vec{r}) = \frac{1}{4\pi\epsilon} \int_V d^3\vec{R} \left( \rho(\vec{R}) \frac{1}{|\vec{d}|} \right), \\
\phi^1(\vec{r}) = \frac{1}{4\pi\epsilon} \int_V d^3\vec{R} \left( \rho(\vec{R}) \frac{d_i}{|\vec{d}|^3} \right), \\
\phi^2(\vec{r}) = \frac{1}{4\pi\epsilon} \int_V d^3\vec{R} \left( q_{ij}(\vec{R}) \frac{3d_i d_j - |\vec{d}|^2 \delta_{ij}}{2|\vec{d}|^5} \right), \\
\phi^3(\vec{r}) = \frac{1}{4\pi\epsilon} \int_V d^3\vec{R} \left( o_{ijk}(\vec{R}) \frac{5d_i d_j d_k - 3|\vec{d}|^2 d_k \delta_{ij}}{2|\vec{d}|^7} \right),
\]

(2.4)

where \( V \) is the total volume of the macroscopic material and \( \vec{d} = \vec{r} - \vec{R} \). The potential \( \phi^0(\vec{r}) \) is due to the free “coarse-grained” charge density in Eq. (2.2). In the limit of \( \nu(\vec{R}) \to 0 \), this coarse grained charge density is the original continuous charge density, and we recover the original expression (2.1). In this case, all other multipole contributions identically vanish.

### 2.2.2 Dependence of the multipole moments on the choice of reference frame

The multipole moments are in general defined with respect to a particular reference frame. For example, given a charge density per unit volume \( \rho(\vec{r}) \), consider the definition of the dipole moment

\[
P_i = \int_v d^3\vec{r} \rho(\vec{r}) r_i.
\]

(2.5)

If we shift the coordinate axes used in that definition by \( \vec{D} \) such that our new positions are given by \( r'_i = r_i + D_i \), and the charge density in this new reference frame is \( \rho'(\vec{r'}) = \rho(\vec{r}) \), the dipole moment is now given by

\[
P'_i = P_i + D_i Q
\]

(2.6)

where \( Q \) is the total charge. Notice, however, that the dipole moment is well defined for any reference frame if the total charge \( Q \) vanishes. Similarly, a quadrupole moment transforms as

\[
Q'_{ij} = Q_{ij} + P_i D_j + D_i P_j + D_i D_j Q
\]

(2.7)

which is not uniquely defined independent of the reference frame unless both the total charge and the dipole moments vanish. In general, for a multipole moment to be independent of the choice of reference frame, all
2.2.3 Boundary properties of multipole moments

Now, let us consider the macroscopic physical manifestations of the multipole moments. In all cases, we will consider the properties that appear at the boundaries of materials having non-vanishing multipole moments in their bulk. We consider each multipole density separately, assuming as indicated above, that all lower moments vanish.

Dipole moment

The potential due to a dipole moment density $p_i(\vec{R})$ is given by the second equation in (2.4). This potential can be recast in the form

$$\phi^1(\vec{r}) = \frac{1}{4\pi\epsilon} \int_{\partial V} d^2\vec{n}(\vec{R}) \left( n_ip_i \frac{1}{|\vec{r} - \vec{R}|} \right) + \frac{1}{4\pi\epsilon} \int_V d^3\vec{R} \left( -\partial_i p_i \frac{1}{|\vec{r} - \vec{R}|} \right).$$  \hspace{1cm} (2.8)

Since both terms scale as $1/|\vec{r} - \vec{R}|$, where $|\vec{r} - \vec{R}|$ is the distance from a point in the material to the observation point, we can define the charge densities

$$\sigma_{\text{face}}(\vec{R}) = n_{i(\alpha)} p_i(\vec{R})$$

$$\rho(\vec{R}) = -\partial_i p_i(\vec{R}).$$  \hspace{1cm} (2.9)

From now on, we will drop the label of the dependence of the variables on $\vec{R}$ for convenience. The first term is the areal charge density on the boundary of a polarized material, and the second term is the volume charge density due to a divergence in the polarization. Hence, one manifestation of the dipole is a boundary charge as shown in Fig. 2.2.
Quadrupole moment

Just as for the dipole contribution, the potential due to a quadrupole moment per unit volume $q_{ij}$ as listed in Eq. (2.4) can be rearranged in terms that scale as $1/d$, where $\vec{d} = \vec{r} - \vec{R}$ is the distance from the point in the material to the observation point, resulting in the charge densities

$$\lambda_{\text{hinge}}^{a,b} = \frac{1}{2} n_i^{(a)} n_j^{(b)} q_{ij},$$

$$\sigma_{\text{face}}^{a} = -\partial_j \left( n_i^{(a)} q_{ij} \right),$$

$$\rho = \frac{1}{2} \partial_j \partial_i q_{ij}. \tag{2.10}$$

The first term is the charge density per length at the hinge $L_{ab}$ of the material. The second term is the area charge density at the boundary surface $S_a$ of the material due to a divergence in the quantity $n_i^{(a)} q_{ij}$. Finally, the third term is the direct contribution of the quadrupole moment density to the volume charge density in the bulk of the material. For a cube with constant quadrupole moment $q_{xy}$ and open boundaries, we illustrate the the charge density in Fig. 2.3(a), as indicated by the expression for $\lambda_{\text{hinge}}$. Notice that the expression for the surface charge density $\sigma_{\text{face}}$ could be written as

$$\sigma_{\text{face}}^{a} = -\partial_j p_j^{\text{face} a}, \tag{2.11}$$

where

$$p_j^{\text{face} a} = n_i^{(a)} q_{ij} \tag{2.12}$$

resembles the polarization for the volume charge density $\rho$ in Eq. (2.9). Thus, we interpret $p_j^{\text{face} a}$ as a bound dipole density (per unit area). This polarization exists on the surface perpendicular to $\hat{n}^{(a)}$ and runs parallel to that surface. An illustration of this polarization for a cube with constant quadrupole moment $q_{xy}$ is shown in Fig. 2.3(b).

Notice, from (2.10) and (2.12), that the magnitudes of the hinge charge densities and the face dipole densities have the same magnitude as the quadrupole moment,

$$|\lambda_{\text{hinge}}| = |p_j^{\text{face}}| = |q_{xy}| \tag{2.13}$$

since the implied sums over $i$ and $j$ in the first equation of (2.10) cancel the factor $\frac{1}{2}$, because $q_{xy} = q_{yx}$. 

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Figure 2.3: Boundary properties of a cube with uniform quadrupole moment per unit volume $q_{xy} \neq 0$, $q_{yz} = q_{zx} = 0$. (a) Boundary charge. Red (blue) color represents positive (negative) charge densities per unit length of magnitude $q_{xy}$. (b) Boundary polarization. Arrows represent boundary dipole moment per unit area of magnitude $q_{xy}$. The unit vectors $\hat{n}^{(x)}$, $\hat{n}^{(-y)}$ and $\hat{n}^{(z)}$ are shown in (a) for reference.

Octupole moment

Following a similar procedure as that employed for the dipole and quadrupole moments, the potential due to an octupole moment per unit volume $o_{ijk}$ [Eq. (2.4)] lead to the charge densities

$$
\delta_{\text{corner} \ a,b,c} = \frac{1}{6} n_{i}^{(a)} n_{j}^{(b)} n_{k}^{(c)} o_{ijk}, \tag{2.14}
$$

$$
\lambda_{\text{hinge} \ a,b} = -\frac{1}{2} n_{i}^{(a)} n_{j}^{(b)} \partial_{k} o_{ijk},
$$

$$
\sigma_{\text{face} \ a} = \frac{1}{2} n_{i}^{(a)} \partial_{j} \partial_{k} o_{ijk},
$$

$$
\rho = -\frac{1}{6} \partial_{i} \partial_{j} \partial_{k} o_{ijk}. \tag{2.15}
$$

The new quantity $\delta_{\text{corner} \ a,b,c}$ represents localized charge bound at a corner where the three surfaces normal to $\hat{n}^{(a)}$, $\hat{n}^{(b)}$, and $n^{(c)}$ intersect. Comparing (2.14) with the expressions for dipole and quadrupole moments we see that we can re-write the hinge charge density per unit length and the surface charge density per unit area as

$$
\lambda_{\text{hinge} \ a,b} = -\partial_{k} p_{k}^{\text{hinge} \ a,b},
$$

$$
\sigma_{\text{face} \ a} = \frac{1}{2} \partial_{j} \partial_{k} q_{jk}^{\text{face} \ a}, \tag{2.15}
$$

where

$$
p_{k}^{\text{hinge} \ a,b} = \frac{1}{2} n_{i}^{(a)} n_{j}^{(b)} o_{ijk},
$$

$$
q_{jk}^{\text{face} \ a} = n_{i}^{(a)} o_{ijk}. \tag{2.16}
$$
Figure 2.4: Boundary properties of a cube with uniform octupole moment per unit volume $o_{xyz}$. (a) Corner-localized charges. Red (blue) color represents positive (negative) charges with magnitude $o_{xyz}$. (b) Hinge-localized dipole moments per unit length of magnitude $o_{xyz}$. (c) Surface localized quadrupole moment densities. Purple squares represent quadrupole moments per unit area of magnitude $o_{xyz}$. The unit vectors $\hat{n}^{(a)}$, $\hat{n}^{(-y)}$ and $\hat{n}^{(z)}$ are shown in (c) for reference.

are the polarization per unit length on hinges where surfaces normal to $\hat{n}^{(a)}$ and $\hat{n}^{(b)}$ intersect and the quadrupole moment density per unit area on faces perpendicular to $\hat{n}^{(a)}$, respectively. These manifestations at the boundary are illustrated in Fig. 2.4 for a cube with uniform octupole moment.

Notice, from (2.14) and (2.16), that the magnitudes of the corner charge densities, the hinge dipole densities, and the face quadrupole densities have the same magnitude as the octupole moment,

$$|\delta_{\text{corner}}| = |p_k^{\text{hinge}}| = |q_{jk}^{\text{face}}| = |o_{xyz}|$$

(2.17) since the implied sums over $i$ and $j$ in the first equation of (2.14) and second equation of (2.16) cancel the prefactors of $\frac{1}{6}$ and $\frac{1}{2}$, respectively, because $o_{xyz} = o_{yxz} = o_{zxy} = o_{zxy} = o_{yxz} = o_{yzx}$.

### 2.2.4 Bulk moments vs. boundary moments

In this section, we draw an important distinction between boundary observables arising from the presence of a bulk moments vs. boundary observables arising from “free” moments of lower dimensionality attached to a boundary. The potential confusion is illustrated in Fig. 2.5 where we consider a neutral, insulating material with no free charge in the bulk or boundary so that all charge accumulation is induced by either dipole or quadrupole moments. In Fig. 2.5(a) there is charge accumulation where two boundary polarizations converge at a corner (in 2D) or a hinge (in 3D). These surface dipoles are meant to be a pure surface effect and not due to a bulk moment. In Fig. 2.5(b) there are both surface polarizations and corner/hinge charge accumulation, but this time exclusively due to a quadrupole moment. The phenomenology in both cases is similar, so the natural question is how to distinguish the surface effect in Fig. 2.5(a) from the bulk effect in Fig. 2.5(b).

To be explicit, let us consider the 2D case. We first consider the existence of only boundary-localized
Figure 2.5: Corner charges due to (a) a pair of convergent dipoles and (b) a constant quadrupole. The most general case up to quadrupole expansion will have a superposition of both contributions.

dipole moments. The contribution to charge density due to a dipole moment density \( \vec{p}(\vec{r}) \) is

\[
\rho = -\nabla \cdot \vec{p}, \quad \sigma = \vec{p} \cdot \vec{n}
\]

which is a restatement of (2.9). The first term is the polarization-induced charge density per unit volume of the material, and \( \vec{p} \cdot \vec{n} \) is the charge density per unit area on a boundary surface with unit normal vector \( \vec{n} \) induced by the bulk polarization \( \vec{p} \). For the purpose of calculating the accumulated charge, let us consider an area \( v \) which encloses the corner on which charge is accumulated, as shown by the red circle in Fig. 2.5(a).

To relate the induced charge in this volume to the polarization at its boundary, we use the first equation in (2.18)

\[
Q_{\text{corner}} = \int_v \rho \, dv = \int_v \left( -\nabla \cdot \vec{p} \right) \, dv = -\oint_{\partial v} \vec{p} \cdot d\vec{s}
\]

where in the second line we have applied Stokes’ theorem, and where \( \partial v \) is the boundary of area \( v \). We see from Fig. 2.5(a) that the boundary dipoles \( \vec{p}_1 \) and \( \vec{p}_2 \) puncture the boundary of \( v \). If we treat the polarizations as fully localized on the edge we can write

\[
\vec{p}_1(\vec{r}) = \hat{x} p_1 \delta(\vec{r} - \vec{r}_1), \quad \vec{p}_2(\vec{r}) = \hat{y} p_2 \delta(\vec{r} - \vec{r}_2),
\]

where \( \vec{r}_1 \) and \( \vec{r}_2 \) are shown in Fig. 2.5. Taking into account that the boundary \( \partial v \) has normal vector \( -\hat{x} \) at \( \vec{r}_1 \) and \( -\hat{y} \) at \( \vec{r}_2 \), we have

\[
Q_{\text{corner}} = p_1 + p_2.
\]

In contrast, let us now consider the charge accumulation inside area \( v \) due to a quadrupole moment \( q_{xy} \).
as shown in Fig. 2.5(b). It follows from (2.10) that, in this case, the induced charge is
\[ \rho = \frac{1}{2} \partial_j \partial_i q_{ij}, \]
where summation is implied for repeated indices. The blue region has quadrupole density \( q_{xy} = q_{yx} \neq 0 \), and outside this region is vacuum. The total charge enclosed in the area \( v \) (shown in red) is
\[ Q_{\text{corner}} = \int_v \rho dv = \int_v \left( \frac{1}{2} \partial_j \partial_i q_{ij} \right) dv = \frac{1}{2} \oint_{\partial v} (\partial_i q_{ij}) n_j ds, \]
where in the second line we have applied Stokes’ theorem. Here, \( n_j \) is the \( j \)th component of the unit vector \( \hat{n} \) normal to the boundary \( \partial v \). Since the quadrupole moment density is constant, there are only two places in \( \partial v \) where the derivative \( \partial_i q_{ij} \) does not vanish [see Fig. 2.5(b)]: (i) at \( \vec{r}_1 \) the unit vector normal to the boundary \( \partial v \), and pointing away from the area \( v \), is \( \hat{n} = -\hat{x} \) and \( \int_{\epsilon}^{\epsilon} \partial_y q_{yx} dy = -q_{yx} \), and (ii) at \( \vec{r}_2 \) the unit vector normal to \( \partial v \) pointing away from \( v \) is \( \hat{n} = -\hat{y} \), which leads to \( \int_{\epsilon}^{\epsilon} \partial_x q_{xy} dx = -q_{xy} \). Thus, the corner charge is,
\[ Q_{\text{corner}} = \frac{1}{2} (q_{xy} + q_{yx}) = q_{xy}. \] (2.20)

By comparing Eq. (2.19) with (2.20), we conclude that, in the case of only boundary-localized “free” dipole moments, the corner-localized charge is given by the sum of the converging boundary polarizations, whereas in the case of a bulk quadrupole moment, the magnitude of the corner charge matches the magnitude of the quadrupole moment. Since the boundary polarizations induced from a bulk quadrupole have the same magnitude as the quadrupole itself [see Eq. (2.12)], adding up the two boundary polarizations in a similar way over-counts the corner charge. Heuristically the two boundary polarizations share the corner charge if arising from a bulk quadrupole moment, whereas they both contribute independently if arising from “free” surface polarization. In summary, even though both cases in Fig. 2.5 have edge-localized polarizations converging at a corner of the material, the resulting corner charge is not determined the same way from the boundary polarizations. For example, if we set \( p_1 = p_2 = q_{xy} \) so that the magnitudes of the edge polarizations match in both cases, the case of converging edge polarizations (2.19) gives a corner charge \( Q_{\text{corner}} = 2q_{xy} \), while the case of a uniform quadrupole moment gives a corner charge \( Q_{\text{corner}} = q_{xy} \).

We now generalize the relations between bulk and boundary moments and their associated boundary charges. In 1D the difference between the total charge on the end of the system and the free charge (i.e.,
monopole moment) attached to the end is captured by the dipole moment

$$Q^{\text{end}} - Q^{\text{free}} = p_x. \quad (2.21)$$

In 2D the difference between the total corner charge and that coming from the total surface polarization contributions is determined by the bulk quadrupole moment

$$Q^{\text{corner}} - p_x^{\text{edge}} - p_y^{\text{edge}} = -q_{xy}. \quad (2.22)$$

Finally, in 3D, we can relate the octupole moment to the difference in the corner charge and the total surface quadrupole and total hinge polarization via

$$Q^{\text{corner}} - \left( \sum_{i=x,y,z} p_i^{\text{hinge}} + q_{xy}^{\text{face}} + q_{yz}^{\text{face}} + q_{xz}^{\text{face}} \right) = o_{xyz}. \quad (2.23)$$

We have implicitly assumed in these three equations that the surfaces, hinges, and corners are all associated with positively oriented normal vectors. For simplicity we have also dropped $Q^{\text{free}}$ in the latter two equations: a free corner monopole has to be subtracted from the corner charge.

### 2.2.5 Symmetries of the multipole moments

Since we are primarily interested in cases where the multipole moments are quantized by symmetry, we need to consider their symmetry transformations. A full discussion of all the transformation properties of all of the components of every multipole moment can be done but would take us too far afield, so we only briefly comment on the simplest properties that provide useful physical intuition.

We focus on systems with $d$-dimensional cubic-like symmetries, e.g., the crystal families of orthorhombic, tetragonal, and cubic materials. For a cubic point group, a non-zero, off-diagonal, $2^d$-pole configuration (e.g., $2^0$: 1 for charge, $2^1$ for dipole $p_x$, $2^2$ for quadrupole $q_{xy}$, and $2^3$ for octupole $o_{xyz}$) is only invariant under the $d$-dimensional “tetrahedral” subgroup ($T(d)$) of the $d$-dimensional cubic symmetry group ($O(d)$).

In 1D, $T(1)$ is just the identity operation. In 2D, $T(2)$ is the normal subgroup of the dihedral group $D_4$ (symmetries of the square) which contains the symmetries $\{1, C_4 M_x, C_4 M_y, C_4^2 \}$, where $M_x, M_y$ are a reflections of only the $x$ and $y$ coordinate, respectively, and $C_4$ is the rotation by $\pi/2$. The quadrupole moment $q_{xy}$ is invariant under $T(2)$. In 3D, $o_{xyz}$ is invariant under the tetrahedral subgroup ($T(3) = T_d$) of the cubic group ($O(3) = O$).

Since the subgroup which leaves the $2^d$-pole invariant is a normal subgroup, we can consider the coset
The trivial element of this coset represents all of the elements of $T(d)$, i.e., the ones that leave the multipole moment invariant. The nontrivial element represents the other transformations in $O$, all of which will cause the off-diagonal $2^d$-poles to switch sign. In 1D, this is simple, as the full symmetry group is just $G = \{1, M_x\}$, and the polarization is invariant only under 1, so $G/1 = G \equiv Z_2$. In conclusion, under a symmetry in $G$ that projects onto the non-identity element of the $Z_2$ factor group, the $2^d$-pole of a crystal insulator should be quantized. In addition, charge conjugation, $C$, quantizes the $2^d$-pole moment (note that each moment depends linearly on the charge). Under these symmetries, the moment is odd and is hence required to either vanish or be quantized to a nontrivial value allowed by the presence of the lattice.

Having defined the multipole moment densities in continuum electromagnetic theory, and having characterized their important observable properties, we now move to describe how they arise in crystalline insulators. We start with a review of dipole moments in 1D crystals, and sequentially advance our description towards bulk and edge dipole moments in 2D crystals, quadrupole moments in 2D crystals, and finally octupole moments in 3D crystals. Due to the dependence of the multipole moments on the origin of coordinates when lower multipole moments do not vanish, we assume in what follows that, for any multipole moment in question, all lower multipole moments vanish.

### 2.3 Bulk dipole moment in 1D crystals

Neutral one-dimensional crystals only allow for a dipole moment. In insulators, the electronic contribution to the polarization\(^1\) arises from the displacement of the electrons with respect to the ionic positive charges. In this section, to calculate the polarization, we diagonalize the electronic projected position operator \([14, 71, 65, 67]\), and construct the Wannier centers and Wannier functions \([72, 73]\). The polarization can then be easily extracted. In doing so, we will recover the result that the electronic polarization is given by the Berry phase accumulated by the parallel transport of the subspace of occupied bands across the Brillouin zone (BZ). The electronic polarization can have a topological nature in the presence of certain symmetries \([4, 8]\).

#### 2.3.1 Preliminary considerations

Let us first consider insulators with discrete translation symmetry, but simply composed of point charges. As seen in Sec. 2.2.2, the polarization is well defined only if it has zero net charge. Discrete translation symmetry implies that it is sufficient to characterize the polarization by considering a single unit cell. Thus, given a definition of a unit cell, and a coordinate frame fixed within it, the dipole moment density per unit

\(^1\)Throughout this paper we will use the terms “polarization” and “dipole moment” interchangeably.
Figure 2.6: Ambiguity in the definition of the electronic positions. Two 1D lattices with one atomic site (blue dots) and one electron (red circles) per unit cell. Although the two physical configurations for the two 1D lattices are the same, the electronic positions $r$ and $r' = r - a$ differ by a lattice constant due to the difference in the definitions of their unit cells.

The length is given by

$$p = \frac{1}{a} \left( \sum_{\alpha=1}^{N_{\text{nuclei}}} q_\alpha R_\alpha + \sum_{\alpha=1}^{N_{\text{elec}}} -e r_\alpha \right), \quad (2.24)$$

where $R_\alpha$ are the positions of the positive charges (i.e., the atomic nuclei), $r_\alpha$ are the electronic positions, and $a$ is the lattice constant (from now on, we will set $a = 1$ for simplicity, unless otherwise specified). We are free to reposition the coordinate frame so that its origin is at the center of charge of the atomic nuclei, i.e., at

$$R_c = \frac{1}{Q_{\text{nuclei}}} \sum_{\alpha=1}^{N_{\text{nuclei}}} q_\alpha R_\alpha, \quad (2.25)$$

where $Q_{\text{nuclei}} = \sum_{\alpha=1}^{N_{\text{nuclei}}} q_\alpha$ is the total positive charge within the unit cell. This choice of coordinate frame cancels out the contribution to the polarization density due to positive charges. Although the coordinate frame is now fixed, there is still an ambiguity in the definition of the unit cell, as illustrated in Fig. 2.6, where the same lattice charge configuration is shown with two definitions of the unit cell. In both cases the locations of both ionic centers (blue dots) and electrons (red circles) are the same, but the electronic positions relative to the ionic charges in the same cell (black arrows), $r$ and $r'$, differ by a lattice constant, i.e., $r' = r - a$. This difference has no physical meaning, and thus the ambiguity is removed by making the identification

$$r_\alpha \equiv r_\alpha \mod a, \quad (2.26)$$

where $a$ is the lattice constant.
With this important subtlety in mind, we now describe the quantum mechanical theory of electronic polarization in crystals developed by King-Smith, Vanderbilt, and Resta [8, 9, 12]. This theory characterizes the bulk dipole moment and is commonly known as the modern theory of polarization. At the core, the approach is as follows: since the electronic wave functions are distributed over the material, we calculate their positions by solving for the eigenvalues of the periodic position operator $\hat{x}$ projected into the subspace of occupied bands [65, 67]. These eigenvalues, or Wannier centers [72], will then map the quantum mechanical problem into the classical problem of point charges [9]. Notably, we find that the eigenfunctions associated to these centers are useful in the formulation of higher multipole moments, as we will see for the case of quadrupole (Sec. 2.6) and octupole (Sec. 2.7) moments.

### 2.3.2 Large Wilson loop, Wannier centers, and Wannier functions

The position operator for the electrons in a crystal with $N$ unit cells and $N_{orb}$ orbitals per unit cell is [71]

$$\hat{x} = \sum_{R,\alpha} c_{R,\alpha}^\dagger |0\rangle e^{-i\Delta_k(R+r_\alpha)} \langle 0| c_{R,\alpha},$$

(2.27)

where $\alpha \in 1 \ldots N_{orb}$ labels the orbital, $R \in 1 \ldots N$ labels the unit cell, $r_\alpha$ is the position of orbital $\alpha$ relative to the center of positive charge within the unit cell or, more generally, relative to the (fixed) origin of system of coordinates (see Sec. 2.3.1), and $\Delta_k = 2\pi/N$ (remember we have set $a = 1$). Taking its Fourier transform, we can alternatively write the position operator as

$$\hat{x} = \sum_{k,\alpha} c_{k+\Delta_k,\alpha}^\dagger |0\rangle \langle 0| c_{k,\alpha},$$

(2.28)

The second quantized Hamiltonian

$$H = \sum_k c_{k,\alpha}^\dagger [h_k]^{\alpha,\beta} c_{k,\beta},$$

(2.29)

can be diagonalized as

$$[h_k]^{\alpha,\beta} = \sum_{n} [u_{nk}^n]^{\alpha} \epsilon_{n,k} [u_{nk}^n]^{\beta},$$

(2.30)

where $[u_{nk}^n]^{\alpha}$ is the $\alpha$-th component of the eigenstate $|u_{nk}^n\rangle$. We can then write Eq. (2.29) as

$$H = \sum_{n,k} \gamma_{n,k}^\dagger \epsilon_{n,k} \gamma_{n,k},$$

(2.31)
where $\gamma_{n,k} = \sum_{\alpha} [u_k^{m\alpha}]^n c_{k,\alpha}$. As we are interested in insulators at zero temperature, we will focus on the occupied electron bands. We hence build the projection operator into occupied energy bands

$$P_{\text{occ}} = \sum_{n=1}^{N_{\text{occ}}} \sum_k \gamma_{n,k}^\dagger \langle 0 | \langle 0 | \gamma_{n,k}, \quad (2.32)$$

where $N_{\text{occ}}$ is the number of occupied energy bands. From now on, we assume that summations over bands include only occupied energy bands. We now proceed to diagonalize the position operator projected into the subspace of occupied bands [71]

$$P_{\text{occ}} \hat{^x} P_{\text{occ}} = \sum_{m,n=1}^{N_{\text{occ}}} \sum_k \gamma_{m,k+\Delta_k}^\dagger \langle 0 | \langle u_{k+\Delta_k}^m | u_k^n \rangle \gamma_{n,k}, \quad (2.33)$$

where we have adopted the notation $\langle u_{k}^m | u_{k}^n \rangle = \sum_{\alpha} [u_k^{m\alpha}]^n [u_k^{n\alpha}]^m \langle u_k^{m\alpha} | u_k^{n\alpha} \rangle \neq \delta_{m,n} \delta_{k,q}$ in general; they only obey $\langle u_{k}^m | u_{k}^n \rangle = \delta_{m,n}$.

The matrix $G_k$ with components $[G_k]^{mn} = \langle u_{k+\Delta_k}^m | u_k^n \rangle$ is not unitary due to the discretization of $k$. However, it is unitary in the thermodynamic limit. To render it unitary for finite $N$, consider the singular value decomposition [74]

$$G = UDV^\dagger, \quad (2.34)$$

where $D$ is a diagonal matrix. The failure of $G$ to be unitary is manifest in the fact that the (real-valued) singular values along the diagonal of $D$ are less than 1. Therefore, we define, at each $k$,

$$F = UV^\dagger \quad (2.35)$$

which is unitary. We refer to $F_k$ as the Wilson line element at $k$. In the thermodynamic limit, $N \to \infty$, we have that $[F_k]^{mn} = [G_k]^{mn}$. To diagonalize the projected position operator, let us write the eigenvalue problem:

$$(P_{\text{occ}} \hat{^x} P_{\text{occ}}) |\Psi^j\rangle = E^j |\Psi^j\rangle, \quad (2.36)$$
which, in the basis $\gamma_{n,k}|0\rangle$, adopts the following form

$$
\begin{pmatrix}
0 & 0 & 0 & \ldots & F_{kN} \\
F_{k_1} & 0 & 0 & \ldots & 0 \\
0 & F_{k_2} & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & 0 \\
\end{pmatrix}
\begin{pmatrix}
\nu_{k_1} \\
\nu_{k_2} \\
\nu_{k_3} \\
\vdots \\
\nu_{k_N} \\
\end{pmatrix}
= E^j
\begin{pmatrix}
\nu_{k_1} \\
\nu_{k_2} \\
\nu_{k_3} \\
\vdots \\
\nu_{k_N} \\
\end{pmatrix},
$$

(2.37)

where $k_1 = 0$, $k_2 = \Delta_k$, $\ldots$, $k_N = \Delta_k(N - 1)$, and $j \in 1\ldots N_{occ}$. Here we have replaced $G_k$ in Eq. (2.36) by $F_k$ to restore the unitary character of the Wilson line elements. By repeated application of the equations above, one can obtain the relation

$$
W_{k_f \leftarrow k_i} |\nu^i_{k_i}\rangle = (E_j)^{(k_f - k_i)/\Delta_k} |\nu^i_{k_f}\rangle,
$$

(2.38)

where we are adopting the bra-ket notation $|\nu^i_{k_i}\rangle$ for the vector formed by the collection of values $[\nu^i_{k_i}]^n$, for $n \in 1\ldots N_{occ}$. We define the discrete Wilson line as

$$
W_{k_f \leftarrow k_i} = F_{k_f - \Delta_k} F_{k_f - 2\Delta_k} \cdots F_{k_i + \Delta_k} F_{k_i}
$$

(2.39)

For a large Wilson loop, i.e. a Wilson line that goes across the entire Brillouin zone (from now on, by Wilson loop we refer exclusively to large Wilson loops), Eq. (2.38) results in the eigenvalue problem

$$
W_{k+2\pi \leftarrow k} |\nu^i_k\rangle = (E^j)^N |\nu^i_k\rangle,
$$

(2.40)

where the subscript $k$ labels the starting point, or base point, of the Wilson loop. While the Wilson-loop eigenstates depend on the base point, its eigenvalues do not. Furthermore, since the Wilson loop is unitary, its eigenvalues are simply phases

$$
(E^j)^N = e^{i2\pi \nu^i}
$$

(2.41)

which has $N$ solutions

$$
E^{j,R} = e^{i2\pi \nu^i/N + i2\pi R/N}
$$

$$
= e^{i\Delta_k(\nu^i + R)}
$$

(2.42)
for \( R \in 0 \ldots N - 1 \). The phases \( \nu^j \) are the Wannier centers. They correspond to the positions of the electrons relative to the center of the unit cells. The eigenfunctions of the Wilson loop at different base points are related to each other (up to a \( U(1) \) gauge, which we now fix to be the identity) by the parallel transport equation

\[
\left| \nu^j_{k_f} \right\rangle = e^{-i(k_f - k_i)\nu^j W_{k_f - k_i}} \left| \nu^j_{k_i} \right\rangle,
\]

which is a restatement of Eq. (2.38). Since \( j \in 1 \ldots N_{\text{occ}} \) and \( R \in 0 \ldots N - 1 \), there are as many projected position operator eigenstates and eigenvalues as there are states in the occupied bands. Given the normalized Wilson-loop eigenstates, the eigenstates of the projected position operator, which now reads as

\[
(P^{\text{occ}}_x P^{\text{occ}}_y) \left| \Psi^j_R \right\rangle = e^{i\Delta_k (\nu^j + R)} \left| \Psi^j_R \right\rangle
\]

are

\[
\left| \Psi^j_R \right\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N_{\text{occ}}} \sum_k \left[ \nu^j_k \right]^n e^{-ikR} \gamma_{nk}^\dagger |0\rangle,
\]

where \( \left[ \nu^j_k \right]^n \) is the \( n^{\text{th}} \) component of the \( j^{\text{th}} \) Wilson-loop eigenstate \( \left| \nu^j_k \right\rangle \). This form of the solution follows directly from (2.37). We call these functions the Wannier functions. Here, \( j \in 1 \ldots N_{\text{occ}} \) labels the Wannier function and \( R \in 0 \ldots N - 1 \) identifies the unit cell to which they are associated. These states obey

\[
\left\langle \Psi^i_{R_1} \left| \Psi^j_{R_2} \right\rangle = \delta_{i,j} \delta_{R_1,R_2},
\right.

i.e., they form an orthonormal basis of the subspace of occupied bands of the Hamiltonian. Before using these results to calculate the polarization, let us comment on the gauge freedom of the Wannier functions. If \( \left| \nu^j_{k_0} \right\rangle \) is the eigenstate of \( W_{k_0 + 2\pi - k_0} \), then so is \( e^{i\phi_0} \left| \nu^j_{k_0} \right\rangle \). Naively, one could assign different phases \( e^{i\phi_k} \) to each of the \( \left| \nu^j_k \right\rangle \) in the expansion of (2.45). However, this is not allowed, because the phases of the Wilson-loop eigenstates at subsequent crystal momenta \( k \) are fixed to \( e^{i\phi_0} \) by the parallel transport relation (2.43)–which is our gauge-fixing condition. Thus, the Wannier functions (2.45) inherit only an overall phase factor \( e^{i\phi_0} \), as expected.
2.3.3 Polarization

The prescription detailed above for the diagonalization of $P_{\text{occ}} \hat{x} P_{\text{occ}}$ reveals that the expected value of the electronic positions relative to the center of positive charge within the unit cell is given by the Wannier centers, which are encoded in the phases of the Wilson-loop eigenvalues, i.e., in

$$W_{k+2\pi-k} |\nu_j^k\rangle = e^{i2\pi\nu_j^k} |\nu_j^k\rangle.$$  \hspace{1cm} (2.47)

For $j = 1 \ldots N_{\text{occ}}$, the Wannier centers are the collection of values $\{\nu_j^k\}$. There are $N_{\text{occ}}$ Wannier centers associated to each unit cell, and there are $N_{\text{occ}}$ electrons per cell in the ground state. The electronic contribution to the dipole moment, measured as the electron charge times the displacement of the electrons from the center of the unit cell is proportional to

$$p = \sum_j \nu_j^k.$$  \hspace{1cm} (2.48)

In the expression above we have set the electron charge $e = 1$. For convenience we will continue to set $e = 1$ in the remainder of the paper, unless otherwise noted. The expression (2.48) is true for any unit cell due to translation invariance, and thus it is a bulk property of the crystal. Since the Wannier centers are the phases of the eigenvalues of the Wilson loop, we can alternatively write the polarization as

$$p = -\frac{i}{2\pi} \log \det [W_{k+2\pi-k}].$$  \hspace{1cm} (2.49)

Furthermore, in the thermodynamic limit, if we write the Wilson loop in terms of the Berry connection

$$[A_k]_{mn} = -i \langle u^n_k | \partial_k | u^m_k \rangle,$$  \hspace{1cm} (2.50)

we have

$$p = -\frac{i}{2\pi} \log \det \left[ e^{-i \int_k^{k+2\pi} A_k dk} \right]$$

$$= -\frac{1}{2\pi} \int_k^{k+2\pi} \text{Tr} [A_k] dk \mod 1,$$  \hspace{1cm} (2.51)

which is the well known expression for the polarization in the modern theory of polarization [8, 9, 12].

The electronic polarization is proportional to the Berry phase that the subspace of occupied bands $P_{\text{occ}} = |u^n_k\rangle \langle u^n_k|$ accumulates as it is parallel-transported around the BZ.
Polarization and gauge freedom

If the electrons are “reassigned” to new unit cells, the polarization changes by an integer (see Fig. 2.6). Mathematically, this is evident in (2.49) from the fact that the Wannier centers $\nu^j$, defined as the log of a $U(1)$ phase, are also defined mod 1. In the expression (2.51) this ambiguity appears because this expression for the polarization is not gauge invariant. One is free to choose a different “gauge” for the functions $|u^m_n\rangle$:

$$|u^m_n\rangle = \sum_n [U^m_n] |u^n_k\rangle.$$ (2.52)

The gauge transformation leads to a new connection

$$A'_k = U^U_k A_k U_k - iU^U_k \partial_k U_k.$$ (2.53)

This new adiabatic connection gives a polarization

$$p' = p + \frac{i}{2\pi} \int^{k+2\pi}_k dk \text{Tr} \left[ U^U_k \partial_k U_k \right]$$

$$= p + \frac{i}{2\pi} \int^{k+2\pi}_k dk \text{Tr} \left[ \partial_k \ln U_k \right]$$

$$= p + \frac{i}{2\pi} \ln \left[ \text{det} U_k \right]^{k+2\pi}_k$$

$$= p + \frac{i}{2\pi} \sum \{ i\phi_i(k + 2\pi) - i\phi_i(k) \}$$

$$= p + n,$$ (2.54)

where $n$ is an integer. The second to last line, $\{ \phi_i(k) \}$ are the phases of the eigenvalues of $U_k$. The fact that $U_k$ is periodic in $k$ implies that the phases of its eigenvalues can differ at most by a multiple of $2\pi$ between $k$ and $k + 2\pi$. Thus, we see that different gauge choices may vary the polarization, but only by integers.

In what follows we will use the Wilson loop formulation of the polarization instead of the expression (2.51) written in terms of the gauge-dependent Berry connection. We will later see that the formulation in terms of Wilson loops has a key additional advantage: the Wilson-loop eigenfunctions give us access to the Wannier functions (2.45), which in turn allow us to generalize the concept of a quantized dipole moment, as discussed in the next subsection, to quantized higher multipole moments.
2.3.4 Symmetry protection and quantization

The polarization can be restricted to specific values in the presence of symmetries. For example, a two-band inversion-symmetric insulator at half-filling has only one electron per unit cell. Thus, the electron center of charge has to be located at either the atomic center or halfway between centers, as any other position of the electron violates inversion symmetry. We say that in this case the polarization is “quantized” to be either 0, for electrons at atomic sites, or \( \frac{1}{2} \), for electrons in between atomic sites. In what follows, we show how symmetries impose constraints on the allowed values of the Wannier centers and consequently on the polarization. We first define the notation for Wilson loops. We denote a Wilson loop with base point \( k \), and with parallel transport towards increasing values of momentum until reaching \( k + 2\pi \) as

\[
W_{x,k} \equiv F_{k+N\Delta k} F_{k+(N-1)\Delta k} \cdots F_{k+\Delta k} F_k,
\]  

(2.55)

where \( F_k \) is the unitary matrix resulting from the singular value decomposition of \( G_k \), which has components \( [G_k]_{mn} = \langle u_{k+\Delta k}^m | u_k^n \rangle \) (see Sec. 2.3.2). Similarly, denote the Wilson loop with base point \( k \) that advances the parallel transport towards decreasing values of momentum until reaching \( k - 2\pi \) as

\[
W_{-x,k} \equiv F_{k-N\Delta k} F_{k-(N-1)\Delta k} \cdots F_{k-\Delta k} F_k.
\]  

(2.56)

These Wilson loops obey

\[
W_{-x,k} = W_{x,k}^\dagger
\]  

(2.57)

We now show the quantization of the polarization in 1D crystals due to inversion and chiral symmetries.

**Inversion symmetry**

A crystal with inversion symmetry obeys

\[
\hat{I} h_{k} \hat{I}^{-1} = h_{-k},
\]  

(2.58)

where \( \hat{I} \) is the unitary (\( \hat{I}^{-1} = \hat{I}^\dagger \)) inversion operator. In the presence of inversion the Wilson loops obey

\[
B_{\hat{I},k} W_{x,k} B_{\hat{I},k}^\dagger = W_{x,-k}^\dagger
\]  

(2.59)
where $B_{m,n}^{m,n} = \langle u_m^n | \hat{I} | u_{-k}^n \rangle$ is the unitary sewing matrix that connects the states at $|u_k^m\rangle$ and $|u_{-k}^m\rangle$ having equal energies. Since the Wilson-loop eigenvalues are independent of the base point, Eq. (2.59) implies that the set of Wilson-loop eigenvalues has to be equal to its complex conjugate, which implies, for the set of Wannier centers,

$$\{\nu_j\} \equiv \{-\nu_j\} \mod 1. \quad (2.60)$$

This forces the Wannier centers to be either 0, $\frac{1}{2}$, or to come in pairs $\{\nu, -\nu\}$. Physically, inversion symmetry implies that the electrons have to either be: (i) centered at an atomic site ($\nu = 0$), (ii) in between sites ($\nu = \frac{1}{2}$), or (iii) to come in pairs arranged on opposite sides of each atomic center and equally distant from it ($\{\nu, -\nu\}$). In the first and third cases, the polarization is 0, while in the second case it is $\frac{1}{2}$. Hence, in general, we have that

$$p \equiv -p \mod 1. \quad (2.61)$$

That is, under inversion,

$$p \equiv 0 \text{ or } \frac{1}{2}. \quad (2.62)$$

This quantization under inversion symmetry allows for an alternative way of calculating the Wannier centers. From (2.58) it follows that at the inversion-symmetric momenta $k^* = 0, \pi$ we have

$$[\hat{I}, h_{k^*}] = 0. \quad (2.63)$$

Thus, the eigenstates of the Hamiltonian at $k^*$ can be chosen to be simultaneous eigenstates of the inversion operator

$$\hat{I} |u_{k^*}\rangle = \mathcal{I}(k^*) |u_{k^*}\rangle, \quad (2.64)$$

where $\mathcal{I}(k^*)$ are the inversion eigenvalues at momenta $k^* = 0, \pi$. The inversion eigenvalues can then be used as labels for the inversion representation at $k^*$ that the occupied bands take. If the representation is the same at $k = 0$ and $\pi$, the topology is trivial, and the polarization is zero. However, if the representations at these two points of the BZ differ, we have a nontrivial topology associated with a non-zero polarization [32, 18, 19].

28
\begin{table}[h]
\centering
\begin{tabular}{ccc}
\hline
I eigenval. & I eigenval. & W eigenval. \\
\hline
at $k = 0$ & at $k = \pi$ & \\
$+$ & $+$ & $+1$ \\
$+$ & $-$ & $-1$ \\
\hline
\end{tabular}
\caption{Relation between inversion and Wilson-loop eigenvalues for an insulator with one occupied band. $\hat{I}$ is the inversion operator. $W$ is the Wilson loop. The signs $\pm$ represent $\pm 1$.}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{ccc}
\hline
$\hat{I}$ eigenval. & $\hat{I}$ eigenval. & W eigenval. \\
\hline
at $k = 0$ & at $k = \pi$ & \\
$(++)$ & $(++)$ & $\{+1, +1\}$ \\
$(++)$ & $(+-)$ & $\{+1, -1\}$ \\
$(++)$ & $(-_-)$ & $\{-1, -1\}$ \\
$(+-)$ & $(+-)$ & $\{\text{c.c.}\}$ \\
\hline
\end{tabular}
\caption{Relation between inversion and Wilson-loop eigenvalues for an insulator with two occupied bands. $\hat{I}$ is the inversion operator. $W$ is the Wilson loop. The signs $\pm$ represent $\pm 1$. c.c. stands for complex conjugate pair of values of magnitude 1.}
\end{table}

We can encode these relations in the expression

$$e^{i2\pi p} = \hat{I}(0)\hat{I}(\pi). \quad (2.65)$$

A formal and complete derivation of the relation between Wilson-loop eigenvalues and inversion eigenvalues was first shown in Ref. [67]. The relations between inversion and Wilson-loop eigenvalues that we will use are shown in Tables 2.1 and 2.2.

**Chiral symmetry**

Although less evident, chiral (sublattice) symmetry also quantizes the polarization. Chiral symmetry implies that the Bloch Hamiltonian obeys

$$\hat{\Pi}h_k\hat{\Pi}^{-1} = -h_k, \quad (2.66)$$

where $\hat{\Pi}$ is the unitary ($\hat{\Pi}^{-1} = \hat{\Pi}^\dagger$) chiral operator. Under this symmetry, the Wilson loop obeys

$$B_{\Pi,k}\mathcal{W}_{k}^{\text{occ}}B_{\Pi,k}^{\dagger} = \text{chiral} \mathcal{W}_{k}^{\text{unocc}}. \quad (2.67)$$

Here, $\mathcal{W}_{k}^{\text{occ}}$ ($\mathcal{W}_{k}^{\text{unocc}}$) is the Wilson loop at base point $k$ over occupied (unoccupied) bands, and $B_{\Pi,k}^{mn} = \langle u^m_k | \hat{\Pi} | u^n_k \rangle$ is a sewing matrix that connects states $|u^m_k\rangle$ and $|u^n_k\rangle$ having opposite energies, that is, such
that $\epsilon_{m,k} = -\epsilon_{n,k}$. Eq. (2.67) implies that the Wannier centers from the occupied bands $\nu_j$ equal those calculated from the unoccupied bands $\eta_j$,

$$\{\nu_j\}^{\text{chiral}} = \{\eta_j\} \mod 1 \quad (2.68)$$

and thus,

$$p^{\text{occ chiral}} = p^{\text{unocc}}. \quad (2.69)$$

It is important to recall that to have strict chiral symmetry as we assume here, the number of occupied bands in a gapped system will be equal to the number of unoccupied bands. To conclude our argument, an additional consideration is necessary: the Hilbert space over all bands (occupied and unoccupied) is topologically trivial. Thus, the polarization that results from both the occupied and unoccupied bands is necessarily also trivial, i.e.,

$$p^{\text{occ}} + p^{\text{unocc}} = 0 \mod 1, \quad (2.70)$$

which leads to

$$p^{\text{occ chiral}} \equiv -p^{\text{unocc}} \mod 1. \quad (2.71)$$

From (2.69) and (2.71) we conclude that

$$p \equiv 0 \text{ or } \frac{1}{2}, \quad (2.72)$$

i.e., the polarization is quantized in the presence of chiral (sublattice) symmetry.

In what follows, we discuss the features of a system with non-zero polarization by studying the minimal model that realizes the dipole phase. In general, a bulk polarization per unit length of $p$ manifests itself at the boundary in the existence of bound surface charges of magnitude $p$, in exact correspondence to the classical electromagnetic theory [cf. Eq. (2.9)]. Consequently, the topological dipole phase exhibits quantized, fractional boundary charge of $\pm \frac{e}{2}$, which can be protected, e.g., by inversion or chiral symmetries. Additionally, we give a concrete example of adiabatic current being pumped in this model [75, 76, 77, 78].
2.3.5 Minimal model with quantized polarization in 1D

A minimal model for an insulator with bulk polarization in one dimension is the Su-Schrieffer-Hegger (SSH) model [13], which describes a chain with alternating strong and weak bonds between atoms, as in polyacetylene [13]. A tight-binding schematic of this structure is shown in Figs. 2.7(a) and 2.7(b). Its Hamiltonian is

\[ H_{\text{SSH}} = \sum_{R} \left( \gamma c_{R,1}^\dagger c_{R,2} + \lambda c_{R,2}^\dagger c_{R+1,1} + \text{H.c.} \right), \]  

(2.73)

where \( \gamma \) and \( \lambda \) are hopping terms within and between unit cells, respectively. Its corresponding Bloch Hamiltonian in momentum space is

\[ h_{\text{SSH}}(k) = \begin{pmatrix} 0 & \gamma + \lambda e^{-ik} \\ \gamma + \lambda e^{ik} & 0 \end{pmatrix}, \]  

(2.74)

where the basis of the matrix follows the numbering in Fig. 2.7(a). More compactly, we will write this, and the Hamiltonians to come, in terms of the Pauli matrices \( \sigma_i \), for \( i = 1, 2, 3 \):

\[ h_{\text{SSH}}(k) = [\gamma + \lambda \cos(k)]\sigma_1 + \lambda \sin(k)\sigma_2. \]  

(2.75)

The SSH model has energies

\[ \epsilon(k) = \pm \sqrt{\lambda^2 + 2\lambda\gamma \cos(k) + \gamma^2}. \]  

(2.76)

The model is gapped unless \( |\gamma| = |\lambda| \). Thus, at half-filling, the SSH model is an insulator, unless \( \gamma = \lambda \) \( (\gamma = -\lambda) \) where the bands touch at the \( k = \pi \) \( (k = 0) \) points of the BZ and the system is metallic.

**Symmetries**

The Hamiltonian (2.74) has inversion symmetry \( \hat{I}h(k)\hat{I}^{-1} = h(-k) \), with \( \hat{I} = \sigma_1 \), and chiral symmetry \( \hat{\Pi}h(k)\hat{\Pi}^{-1} = -h(k) \) with \( \hat{\Pi} = \sigma_3 \). Thus, this model has quantized polarization: \( p = 0 \) for \( |\gamma| > |\lambda| \) and \( p = \frac{1}{2} \) for \( |\gamma| < |\lambda| \). At \( |\gamma| = |\lambda| \), the energy gap closes. This crossing is necessary to change the insulating phase from one with \( p = 0 \) to \( p = \frac{1}{2} \), or vice versa. Thus, the polarization is an index that labels two distinct phases, the ‘trivial’ \( p = 0 \) phase and the ‘nontrivial’ or ‘dipole’ phase \( p = \frac{1}{2} \). This is the simplest example of a symmetry protected topological (SPT) phase, because the two phases are clearly distinguished.
only in the presence of the symmetries that quantize the dipole moment. However, both the trivial and the “nontrivial” state are described in terms of localized Wannier states; therefore, a more appropriate term for the “nontrivial” state is an obstructed atomic limit [49]. An illustration of these two phases and the transition point is shown in Fig. 2.7(c), where the spectrum of the open-boundary Hamiltonian is parametrically plotted as a function of $\gamma$, for a fixed value of $\lambda = 1$.

**Quantization of the boundary charge**

In an SSH crystal with open boundaries, one consequence of the quantization of the bulk polarization to $\frac{e^2}{2}$ in the nontrivial dipole phase is the appearance of $\pm \frac{e^2}{2}$ charge at its edges. This accumulation is due to the existence of two degenerate and edge-localized modes. In the presence of chiral symmetry, the energies of the edge-localized states are pinned to zero. Furthermore, these edge-localized states are eigenstates of the chiral operator. In the absence of chiral symmetry, the zero-energy protection of the edge modes is lost; chiral-breaking terms lift the energies of the edge modes away from 0, but they will remain degenerate (resulting in a twofold-degenerate ground-state at half-filling) as long as inversion symmetry is preserved in the system.

To determine a fixed sign for the polarization, one must weakly break the degeneracy of the edge modes. For $N$ unit cells, half-filling implies that there are $N$ electrons, $N - 1$ of which fill bulk states. The extra electron thus will fill one of the edge states, but if they are degenerate, the electron cannot pick which state to fill. Splitting the degeneracy infinitesimally is enough to decide which end state is filled, thus choosing...
the “sign” of the dipole. In the SSH model, the symmetry breaking can be achieved by adding the term \( \delta \sigma_3 \) to (2.75) for an infinitesimal value of delta \( \delta \). Notice that \( \sigma_3 \) breaks both chiral and inversion symmetries, as required.

### 2.3.6 Charge pumping

In this section, we describe the pumping of electronic charge in insulators by means of adiabatic deformations of the Hamiltonian. Originally conceived by Thouless [7] as a method to extract current out of an insulator, this mechanism also has a well-established connection with the quantum anomalous Hall effect [16]. In what follows, we describe two concrete examples of charge pumping. We start with a pedagogical example that allows us to closely follow the motion of the Wannier centers during the adiabatic evolution. However, this model requires a piecewise continuous parametrization. Therefore we also describe a pumping with a fully continuous parametrization - although it is less obvious pictorially.

The pedagogical example uses the SSH model as follows. Consider the SSH Hamiltonian (2.75) with additional on-site energies \( \delta \sigma_3 \), which breaks the chiral and inversion symmetries,

\[
h_{\text{SSH}}^{\delta}(k) = [\gamma + \lambda \cos(k)] \sigma_1 + \lambda \sin(k) \sigma_2 + \delta \sigma_3.
\]

We modify the parameters \( \lambda, \gamma, \) and \( \delta \) adiabatically:

\[
(\delta, \lambda, \gamma) = \begin{cases} 
(\cos(t), \sin(t), 0) & 0 < t \leq \pi \\
(\cos(t), 0, |\sin(t)|) & \pi < t \leq 2\pi
\end{cases}
\]

where \( t \) is the adiabatic parameter. This parametrization represents an evolution of a family of Hamiltonians through closed cycles that return to the original configuration when \( t = 2\pi p \) for integer \( p \). After each cycle, however, an electron is transferred from the left to the right at each unit cell. The first half of the cycle is illustrated in Fig. 2.8. At \( t = 0 \) the Hamiltonian is \(+\sigma_3\), i.e., it is in the trivial atomic limit, and at half-filling the basis sites “2” are occupied. In Fig. 2.8(a), this corresponds to the north pole of the Bloch sphere. As time progresses, the hopping amplitude \( \lambda \) increases while keeping \( \gamma = 0 \), which results in the wave functions progressively leaking into sites “1” of the neighboring unit cells to their right. At \( t = \pi/2 \) the occupancy of the sites is uniform, with Wannier center in between unit cells. This is the nontrivial dipole phase, with \( p = \frac{1}{2} \). Then, for \( \pi/2 < t < \pi \) the hopping amplitude decreases while the on-site potentials reverse sign. Thus, the eigenstates increasingly occupy states “1”. At \( t = \pi \), the Hamiltonian is \(-\sigma_3\), and only sites “1” are occupied. In Fig. 2.8(a), this corresponds to the south pole of the Bloch sphere. During
Figure 2.8: Adiabatic pumping of an electron in the SSH model [Eq. (2.77)] parametrized by (2.78) during the first half of the cycle. (a) As the adiabatic parameter $t$ advances, the Berry phase of the occupied band across the BZ increases proportional to the solid angle enclosed by the ground-state projector on the Bloch sphere. (b) Electronic positions at $t = 0, \pi/2, \pi$ that illustrate how the positions advance proportionally to the Berry phase illustrated in (a). The second half of the cycle generates no transport and is not illustrated.

This first half of the cycle, electrons have crossed one unit cell to the right. Topologically, the entire Bloch sphere of the Hamiltonian in Eq. (2.77) has been swept, which is characterized by a Chern number $n = 1$. The second half of the cycle does not cause transport, as it switches the electron occupancy from sites “1” back to sites “2” on the same unit cell (since $\lambda = 0$). At $t = 3\pi/2$, the system is again inversion-symmetric, and the occupancy is uniform, with Wannier center in the middle of the unit cell. This is the $p = 0$ phase. Hence, we can think of the above interpolation as an cycle between the $p = \frac{1}{2}$ and the $p = 0$ phases, during which, as explicitly shown, an electron has been moved from one side of the chain to the other.

The pumping method described above has a pictorial representation. Another adiabatic pumping process, less intuitive but which uses a fully continuous parametrization is given by the family of Hamiltonians

$$h(k,t) = [\gamma + \cos(k)]\sigma_1 + \sin(k)\sigma_2 + m\sin(t)\sigma_3 + [1 + m\cos(t)]\sigma_2,$$  \hspace{1cm} (2.79)

where $t$ is the adiabatic parameter. Figure 2.9 shows the energy bands and the Wannier centers as a function of the adiabatic parameter. Equation (2.79) encloses a monopole of Berry flux as it sweeps out a torus $T^2$ instead of a sphere $S^2$ as in (2.78). In Fig. 2.9, $\gamma = 0.5$ and $m = 1$. Thus, at $t = 0$ the system is in the trivial phase, while at $t = \pi$ the lattice is in the SSH dipole phase. Correspondingly, we see that at $t = 0$ there are no zero-energy modes when boundaries are open [Fig. 2.9(a)], and the Wannier center (and consequently its polarization) is at a value of zero [Fig. 2.9(b)]. At $t = \pi$, there are two states with zero energy when we have open boundaries, and the Wannier center is at $\nu = \frac{1}{2}$. Finally, at $t = 2\pi$ the system has returned back to its initial state in the atomic limit after the charge has moved by one unit cell. This process can be used to generate a lattice model in one spatial dimension higher which will be topologically equivalent to a quantum anomalous Hall (Chern) insulator. This is carried out by reinterpreting the adiabatic parameter as an additional momentum quantum number for a 2D system [16]. This connection will become apparent in
Sec. 2.4.

2.4 Bulk dipole moment in 2D crystals

We now investigate the existence of dipole moments in 2D crystals with $N_x \times N_y$ sites. Without loss of generality, we calculate the position operator along $x$ projected into the occupied bands [71]

$$P_{\text{occ}}^x P_{\text{occ}} = \sum_k \gamma^\dagger_{m,(k_x+\Delta_{k_x},k_y)} |0\rangle \left< u_n^{m,(k_x+\Delta_{k_x},k_y)} | u_m^{n,(k_x,k_y)} \right> \langle 0 | \gamma_{n,(k_x,k_y)}$$

(2.80)

which is similar to Eq. (2.33), but with the extra quantum number $k_y$. Importantly, notice that the operator is diagonal in $k_y$. Thus, all the findings in Sec. 2.3 follow through in this case too, but with the extra label $k_y$. In particular, for a large Wilson loop $W_{x,k}$, which has $k = (k_x, k_y)$ as its base point and runs along increasing values of $k_x$, as the obvious extension to 2D of definition (2.55), we have

$$W_{x,k} |\nu_x^j(k_x,k_y)\rangle = e^{i2\pi \nu_x^j(k_x,k_y)} |\nu_x^j(k_x,k_y)\rangle,$$

(2.81)

The Wannier functions along $x$ are then

$$|\Psi_{R_x,k_y}^j\rangle = \frac{1}{\sqrt{N_x}} \sum_{n=1}^{N_{\text{occ}}} \sum_{k_x} \gamma^\dagger_{n,k_x} |0\rangle \left[ \nu_x^j(k_x,k_y) \right]^n e^{-ik_x R_x},$$

(2.82)

where $k = (k_x, k_y)$ is the crystal momentum, with $k_{x,y} = n_{x,y} \Delta_{k_{x,y}}$, for $n_{x,y} \in 0, 1, \ldots, N_{x,y} - 1$ and $\Delta_{k_{x,y}} = 2\pi/N_{x,y}$. These functions obey

$$\langle \Psi_{R_x,k_y}^j | \Psi_{R_x,k_y'}^j \rangle = \delta_{j,j'} \delta_{R_x,R_x'} \delta_{k_y,k_y'},$$

(2.83)
i.e., they form an orthonormal basis of the subspace of occupied energy bands of the Hamiltonian. For the Wilson-loop eigenstates \( |\nu_{x,k}^j\rangle\), the subscript \( x \) specifies the direction of its Wilson loop, and \( k \) specifies its base point, so, for example, Eq. (2.81) is explicitly written as

\[
&W_{(k_x+2\pi,k_y)} \cdot |\nu_{x,k}^j\rangle = (E_j)^N |\nu_{x,(k_x,k_y)}^j\rangle.
\]

(2.84)

Although the phases \( \nu_j^k(k_y) \) of the eigenvalues of the Wilson loop \( W_{x,k} \) do not depend on \( k_x \), in general they do depend on \( k_y \). Thus, the polarization for one-dimensional crystals translates into polarization as a function of \( k_y \) in its 2D counterpart, that is,

\[
p_x(k_y) = \sum_{j=1}^{N_{occ}} \nu_j^k(k_y) = -\frac{i}{2\pi} \text{Log Det}[W_{x,k}],
\]

(2.85)

which, in the thermodynamic limit becomes

\[
p_x(k_y) = -\frac{1}{2\pi} \int_{0}^{2\pi} \text{Tr}[A_{x,k}] dk_x,
\]

(2.86)

where \( k = (k_x, k_y) \) and \([A_{x,k}])_{mn} = -i \langle u_k^m|\partial_{k_x}|u_k^n\rangle\) is the non-Abelian Berry connection (where \( m, n \) run over occupied energy bands). The total polarization along \( x \) is

\[
p_x = \frac{1}{N_y} \sum_{k_y} p_x(k_y).
\]

(2.87)

In the thermodynamic limit, \( \frac{1}{N_y} \sum_{k_y} \rightarrow \frac{1}{2\pi} \int dk_y \), the polarization along \( x \) in 2D crystals is

\[
p_x = -\frac{1}{(2\pi)^2} \int_{BZ} \text{Tr}[A_{x,k}] d^2k.
\]

(2.88)

Here, \( BZ \) is the 2D Brillouin zone. The 2D polarization is thus given by the vector \( p = (p_x, p_y) \), where each component \( p_i \) is calculated using (2.88) with \([A_{i,k}])_{mn} = -i \langle u_k^m|\partial_{k_i}|u_k^n\rangle\), for \( i = x, y \).

### 2.4.1 Symmetry protection and quantization

As in 1D, the polarization in 2D can have the values 0 or \( \frac{1}{2} \) (in appropriate units) under the presence of certain symmetries. In this section, we consider the symmetries that protect the quantization of the polarization in 2D.
Reflection symmetries

In the presence of reflection symmetries $M_x : x \rightarrow -x$ and $M_y : y \rightarrow -y$, the Bloch Hamiltonian obeys

$$\hat{M}_x h(k_x, k_y) \hat{M}_x^{-1} = h(-k_x, k_y), \quad \hat{M}_y h(k_x, k_y) \hat{M}_y^{-1} = h(k_x, -k_y), \quad (2.89)$$

respectively. The polarization along $x$ as a function of $k_y$ (2.86) under these symmetries obeys

$$p_x(k_y) \overset{M_x}{=} -p_x(k_y), \quad p_x(k_y) \overset{M_y}{=} p_x(-k_y), \quad (2.90)$$

and similarly for $p_y(k_x)$. These relations imply that, under $M_x$,

$$p_x(k_y) \overset{M_x}{=} 0 \text{ or } \frac{1}{2} \quad (2.91)$$

(and similarly for $p_y(k_x)$ under $M_y$). This quantized value can be easily computed by comparing the reflection representations at the reflection-invariant lines in the BZ. Concretely, from (2.89) it follows that

$$[\hat{M}_x, h(k_x, k_y)] = 0 \quad (2.92)$$

for $k_{sx} = 0, \pi$ and for $k_y \in [-\pi, \pi)$. Thus, following with the rationale in Sec. 2.3.4 for the case of inversion in 1D, the polarization $p_x(k_y)$ under reflection symmetry $M_x$ can be found by calculating

$$e^{i2\pi p_x(k_y)} = m_x(0, k_y) m_x^*(\pi, k_y). \quad (2.93)$$

where $m_x(k_{sx}, k_y)$ are the reflection eigenvalues at the reflection-invariant lines of the BZ and the asterisk stands for complex conjugation (in the case of double-groups for which reflection operators have complex eigenvalues).

Now, the polarization at fixed $k_y$ can be thought of as the polarization of a 1D Bloch Hamiltonian $h(k_x, k_y)$, for $k_x \in [-\pi, \pi)$. From (2.91), under reflection $M_x$, this 1D Hamiltonian has quantized polarization. Since this polarization is a topological index, a change in this index $p_x(k_y)$ across $k_y$ is only possible if the Hamiltonian $h(k_x, k_y)$ closes the gap at certain values of $k_y$. Thus, for Hamiltonians that are gapped in energy for all $k_x, k_y \in [-\pi, \pi)$, their polarizations $p_x(k_y)$ are not only quantized, but also continuous across
$k_y \in [-\pi, \pi)$. This implies that the overall polarization is also quantized,

$$p_i \equiv 0 \text{ or } \frac{1}{2}$$

(2.94)

for $i = x, y$.

**Inversion symmetry**

Under inversion symmetry, the Bloch Hamiltonian obeys

$$\hat{I}h_k\hat{I}^{-1} = h_{-k}.$$  

(2.95)

In 2D, this equation also describes a $C_2$ symmetry, $\hat{r}_2 h_k\hat{r}_2^{-1} = h_{-k}$, where $\hat{r}_2$ is the $C_2$ rotation operator.

The difference is that, for spinful systems, $\hat{r}_2^2 = -1$, while $\hat{I}^2 = 1$. For convenience, we will only refer to inversion symmetry ($\hat{I}$) in what follows. The conclusions in this section, however, apply to both $\hat{I}$ and $C_2$ symmetries.

Under inversion symmetry, we have the relation

$$p_x(k_y) \overset{\text{I}}{=} -p_x(-k_y) \mod 1.$$  

(2.96)

This implies that the polarization (2.87) obeys

$$p_x \overset{\text{I}}{=} -p_x \mod 1,$$  

(2.97)

i.e., under inversion symmetry the polarization is quantized:

$$p_x \overset{\text{I}}{=} 0 \text{ or } \frac{1}{2}.$$  

(2.98)

However, the restriction (2.96) does not quantize the polarization at each $k_y$, as in (2.91) for reflection symmetries. This allows for $p_x(k_y)$ to acquire any value $[0, 1]$, except at the inversion symmetric momenta $k_{sy} = 0, \pi$, where we have

$$p_x(k_{sy}) \overset{\text{I}}{=} 0 \text{ or } \frac{1}{2}.$$

(2.99)

The two values, $p_x(0)$ and $p_x(\pi)$, are topological indices that are related to the parity of the Chern
In the presence of reflection symmetries $M_x$ and $M_y$ and inversion $I$, the Hamiltonian at the solid blue (dashed red) lines commutes with $\hat{M}_x (\hat{M}_y)$. At the points $\Gamma = (0, 0)$, $X = (\pi, 0)$, $Y = (\pi, 0)$, and $M = (\pi, \pi)$ the Hamiltonian also commutes with $\hat{I}$.

number [defined in Eq. (2.107)] [18, 19]

$$e^{i\pi n} = e^{i2\pi p_x(0)}e^{i2\pi p_x(\pi)}.$$  \hspace{1cm}  (2.100)

This relationship between the parity of the Chern number and the polarizations $p_x(0)$, $p_x(\pi)$ will become apparent in the discussion to follow in Sec. 2.4.2. Using (2.65), this expression reduces to

$$e^{i\pi n} = I(\Gamma)I^*(X)I(Y)I^*(M),$$  \hspace{1cm}  (2.101)

where the momenta $\Gamma$, $X$, $Y$, and $M$ are shown in Fig. 2.10. Since the inversion eigenvalues are real for both single and double groups, complex conjugation is not necessary if $I(k_\star)$ is an inversion eigenvalue. However, we have added complex conjugation to accommodate for the case in which $C_2$ symmetry is considered instead, for which its eigenvalues are complex for double groups.

The polarization of an insulator with a non-zero Chern number is a subtle matter and requires special care because of the partial occupation of the chiral edge states [79]. We will only consider the polarization of insulators with vanishing Chern number. When the Chern number is zero, the polarization can be determined from the inversion eigenvalues of the occupied bands via [18, 19]

$$p_x \triangleq \begin{cases} 0 & \text{if } I(\Gamma)I^*(X) = +1 \text{ and } I(Y)I^*(M) = +1, \\ \frac{1}{2} & \text{if } I(\Gamma)I^*(X) = -1 \text{ and } I(Y)I^*(M) = -1. \end{cases}$$  \hspace{1cm}  (2.102)

For a system with vanishing Chern number, the polarization $p_x(k_y)$ for $k_y = 0$ and $\pi$ are identical. Hence we only need to compare either $I(\Gamma)$ and $I(X)$ together or $I(Y)$ and $I(M)$ together to determine $p_x$. Similarly,
Figure 2.11: A weak topological insulator formed by stacking 1D insulators in the topological dipole phase. (a) Lattice. (b) Inversion eigenvalues at the high-symmetry points Τ, X, Y, and M.

$p_y$ can be inferred by

\[
p_y = \begin{cases} 
0 & \text{if } I(\Gamma)I^*(Y) = +1 \text{ and } I(X)I^*(M) = +1 \\
\frac{1}{2} & \text{if } I(\Gamma)I^*(Y) = -1 \text{ and } I(X)I^*(M) = -1 
\end{cases}.
\]

(2.103)

A simple realization of an insulator with polarization \((p_x, p_y) = (\frac{1}{2}, 0)\) is shown in Fig. 2.11(a), which consists of a series of 1D SSH chains in the topological dipole phase oriented along \(x\) and stacked along \(y\). It has inversion eigenvalues as shown in Fig. 2.11(b). Such a stacked insulator is called a weak topological insulator (weak TI) [80, 36, 37, 81], because, although it is a 2D system, its nontrivial topology is essentially one-dimensional. Thus, they can be realized by stacking layers of 1D topological insulators. In this particular case the ground state of the system can be described by localized Wannier states in both the trivial and nontrivial phases, and hence we could again identify it with an obstructed atomic limit [49]. In general, the polarization of a weak TI is described by an index [80, 36, 37]

\[
G = p_x b_y + p_y b_x,
\]

(2.104)

where \(p_x\) and \(p_y\) are the polarizations (2.88), which can be determined by (2.102) and (2.103), and \(b_x, b_y\) are unit reciprocal lattice vectors of the crystal.

In the case of insulators with multiple occupied bands, the single inversion eigenvalue \(I(k)\) in (2.102) and (2.103), for \(k = \Gamma, X, Y, \text{ and } M\), is replaced by the multiplication of the inversion eigenvalues of all the occupied bands at \(k\). For example, consider the two insulators with Bloch Hamiltonians

\[
h^1(k) = [\cos(k_x)\tau_x + \sin(k_x)\tau_y] \oplus [\cos(k_y)\tau_x + \sin(k_y)\tau_y] + \gamma \tau_x \otimes (\tau_0 + \tau_x),
\]

\[
h^2(k) = [\cos(k_x - k_y)\tau_x + \sin(k_x - k_y)\tau_y] \oplus [\cos(k_x + k_y)\tau_x + \sin(k_x + k_y)\tau_y] + \gamma \tau_x \otimes (\tau_0 + \tau_x),
\]

(2.105)
Figure 2.12: Insulator with Bloch Hamiltonian $h^1(k)$ as in the first equation of (2.105). Periodic boundaries are imposed, so that top and bottom edges, as well as left and right edges, are identified. (a) Lattice. Hopping terms (black lines) have strength 1. Couplings within unit cells (red lines) have strength $\gamma \ll 1$. Red circles indicate 2D Wannier centers. (b) Inversion eigenvalues at the high symmetry points $\Gamma$, $X$, $Y$, and $M$. (c) $M_x$ eigenvalues along the $(0, k_y)$ and $(\pi, k_y)$ invariant lines. (d) $M_y$ eigenvalues along the $(k_x, 0)$ and $(k_x, \pi)$ invariant lines.

which have lattices and inversion and reflection eigenvalues as shown in Figs. 2.12 and 2.13, respectively. Their weak indices are $G^1 = (\frac{1}{2}, \frac{1}{2})$ and $G^2 = (0, 0)$, respectively. In the case of $h^1(k)$, the two Wannier centers of the two occupied bands are $\{\nu_x, \nu_y\} = \{0, \frac{1}{2}\}$ and $\{\nu_x, \nu_y\} = \{\frac{1}{2}, 0\}$, as indicated by the red circles in Fig. 2.12(a). This leads to a nontrivial polarization along both directions. In the case of $h^2(k)$, on the other hand, the two Wannier centers have the same value $\{\nu_x, \nu_y\} = \{\frac{1}{2}, \frac{1}{2}\}$, leading to trivial polarization when combined. Notice, from the inversion eigenvalues shown in Fig. 2.13(b), that although $h^2(k)$ has trivial polarization, it is not a trivial atomic limit insulator (a trivial insulator has all inversion eigenvalues at all high symmetry points equal), it is an obstructed atomic limit where the Wannier centers are located away from the atom positions \[49\].

A more comprehensive classification of topological crystalline insulators takes into account the full structure of the inversion eigenvalues of the occupied bands, or, more generally, the point group corepresentations on the subspace of occupied bands, to construct crystalline topological invariants \[26, 27, 28, 29, 30, 31, 32, 18, 19, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50\]. Such a classification, however, is outside of the scope of this paper.

Finally, we point out that the inversion eigenvalues in Figs. 2.12 and 2.13 are compatible with the relations shown in Table 2.2.
Figure 2.13: Insulator with Bloch Hamiltonian $h^2(k)$ as in the second equation of (2.105). Periodic boundaries are imposed, so that top and bottom edges, as well as left and right edges, are identified. (a) Lattice. Hopping terms (black lines) have strength 1. Couplings within unit cells (red lines) have strength $\gamma \ll 1$. Red circles indicate 2D Wannier centers. (b) Inversion eigenvalues at the high symmetry points $\Gamma$, $X$, $Y$, and $M$. (c) $M_x$ eigenvalues along $(0, k_y)$ and $(\pi, k_y)$. (d) $M_y$ eigenvalues along $(k_x, 0)$ and $(k_x, \pi)$.

2.4.2 Wilson loops and Wannier bands

We now introduce the concept of Wannier bands as the set of Wannier centers along $x$ as a function of $k_y$, $\nu_x(k_y)$, or, vice versa, as the set of Wannier centers along $y$ as a function of $k_x$, $\nu_y(k_x)$. Unless otherwise specified, we will use the generic term Wannier bands to refer to $\nu_x(k_y)$. The Wannier bands have associated hybrid Wannier functions (2.82) that are localized along $x$ but are Bloch-like along $y$. Although the term ‘hybrid Wannier function’ is rather general, as more than one definition exists to refer to partially localized states [82, 83, 70, 84], here we refer exclusively to the eigenstates of the projected position operator along one direction as a function of the perpendicular crystal momentum, as in Eq. (2.82). They will be useful in the formulation of higher multipole moments in Sec. 2.6. Figure 2.14 shows the Wannier bands for (a) the insulator $h^1(k)$, (b) the insulator $h^2(k)$, (c) a Chern insulator, and (d) a quantum spin Hall (QSH) insulator. These last two insulators have corresponding Hamiltonians

$$h^{\text{Chern}}(k) = \sin(k_x)\tau_x + \sin(k_y)\tau_y + [m + \cos(k_x) + \cos(k_y)]\tau_z,$$
$$h^{\text{QSH}}(k) = \sin(k_x)(\Gamma_{xx} + \Gamma_{zz}) + \sin(k_y)(\Gamma_{yx} + \Gamma_{0y}) + [2 - m - \cos(k_x) - \cos(k_y)]\Gamma_{0z}, \quad (2.106)$$

where $\Gamma_{ij} = \sigma_i \otimes \tau_j$, and $\sigma_i$ ($\tau_i$) are Pauli matrices corresponding to the spin (orbital) degrees of freedom. We consider these models at half-filling. At this filling, all of them are insulators.
Figure 2.14: Wannier bands in (a) weak topological insulator, (b) trivial insulator, (c) Chern insulator, and (d) QSH insulator. The Wannier band in (b) is twofold degenerate. (a), (b) have Hamiltonians (2.105), respectively. (c), (d) have Hamiltonians (2.106) with $m = 1$ and 3, respectively.

The models $h^1(k)$ and $h^2(k)$, described in Sec. 2.4.1, admit the construction of 2D Wannier centers. Indeed, the electron Wannier centers in these two models can be essentially located by inspection. Specifically, with vanishing couplings within unit cells ($\gamma = 0$), reflection symmetry then implies that, at half-filling (with two electrons per unit cell), the electron positions have to be as shown with red circles in Figs. 2.12(a) and 2.13(a). Having two occupied bands, these insulators have two Wannier bands each. For $h^1(k)$, the $\nu_x(k_y)$ bands are $\nu^1_x(k_y) = 0, \nu^2_x(k_y) = \frac{1}{2}$. These values are fixed by reflection symmetry [Fig. 2.12(c)], and match the electronic positions in Fig. 2.12(a). For $h^2(k)$, we have $\nu^1_x(k_y)$ and $\nu^2_x(k_y)$ coming in opposite pairs. This is allowed by its reflection eigenvalues [Fig. 2.13(c)]. Notice, however, that the inversion eigenvalues in this model [Fig. 2.13(b)] impose certain degeneracies in the Wannier values, $\nu^1_x(0) = \nu^2_x(0) = \frac{1}{2}$ and $\nu^1_x(\pi) = \nu^2_x(\pi) = \frac{1}{2}$. Thus, the two electronic positions have to be degenerate at a value of $\frac{1}{2}$, as shown in the pictorial representation of Fig. 2.13(a). When Wannier bands $\nu_y(k_x)$ are calculated in these two models, we obtain the similar plots.

The case of the Chern insulator and the QSH insulator are not as straightforward to interpret because it is not possible to map the electronic wave functions to “pointlike” charges as in the case of insulators in obstructed atomic limits, such as $h^1(k)$ and $h^2(k)$ [Eq. (2.105)]. In the case of the Chern insulator, the Wannier band $\nu_x(k_y)$ winds around one time across the 1D BZ $k_y \in [0, 2\pi)$. In general, a Chern insulator will wind around $n$ times, where

$$n = \frac{1}{2\pi} \int_{\text{BZ}} d^2k \text{Tr}[\mathcal{F}(k)]$$

(2.107)
is the Chern number of the Chern insulator. Here, \( F(k) = \partial_{k_x} A_{y,k} - \partial_{k_y} A_{x,k} + i[A_{x,k}, A_{y,k}] \) is the Berry curvature. To see how the Chern number encodes this winding of the Wannier bands, let us take the simple case in which \([A_{x,k}, A_{y,k}] = 0\). Furthermore, let us make the gauge choice \( \partial_{k_x} A_{y,k} = 0 \). Then we have

\[
n = \frac{1}{2\pi} \int_{BZ} d^2k \left( -\partial_{k_y} \text{Tr}[A_{x,k}] \right) = \int_0^{2\pi} dk_y \partial_{k_y} p_x(k_y) \tag{2.108}\]

Notice the resemblance of the Wannier band in Fig. 2.14(c) with the Wannier centers as a function of the adiabatic parameter \( t \) in Fig. 2.9(b). Indeed, both insulators are systems with topology indexed by \( n = 1 \); if in Eq. (2.79) we make the change \( t \to k_y \), the system becomes a Chern insulator. The reverse procedure, termed dimensional reduction, is one method for a hierarchical classification of topological insulators [16]. The dimensional reduction mathematically connects the 2D Chern insulator with the adiabatic pumping of charge by means of a changing dipole moment in 1D.

In general, this type of dimensional hierarchy mathematically connects topological insulators of different dimensions, having the dipole moment as its starting point in 1D. However, this connection does not provide a natural physical generalization of the 1D dipole moment to higher multipole moments. In Sec. 2.6 we show that, in order to generate a classification that generalizes the 1D dipole moment to higher multipole moments in higher dimensions, the notion of Wannier bands is useful.

**Symmetry constraints on Wannier bands**

The Wannier bands, being related to the position of electrons in the lattice, are constrained in the presence of symmetries. The constraints due to time reversal (TR), chiral, and charge-conjugation (CC) symmetries are

\[
\{ \nu_x^i(k_y) \} \overset{\text{TR}}{=} \{ \nu_x^i(-k_y) \},
\{ \nu_y^i(k_y) \} \overset{\text{chiral}}{=} \{ \eta_x^i(k_y) \},
\{ \nu_x^i(k_y) \} \overset{\text{CC}}{=} \{ \eta_x^i(-k_y) \} \tag{2.109}
\]

mod 1. In the last two relations, the values \( \{ \eta_x^i(k_y) \} \) are Wannier bands calculated over unoccupied energy bands. The Chern insulator with Hamiltonian as in the first equation of (2.106) breaks TR symmetry, because its Wannier bands [Fig. 2.14(c)] are not symmetric with respect to \( k_y = 0 \), as required by the first Eq. in (2.109). In contrast, the QSH insulator with Hamiltonian as in the second equation of (2.106) shows Wannier bands compatible with TR symmetry [Fig. 2.14(d)] [65, 85, 86]. Indeed, the QSH insulator has nontrivial topology protected by TR symmetry due to Kramers degeneracy. This protection is also manifest
Table 2.3: Relation between eigenvalues of $\hat{Q} = \hat{I}, \hat{M}_x$ or $\hat{M}_y$ and Wilson loops. $\pm$ are the eigenvalues of reflection or inversion operators at high-symmetry momenta $k^*$ and $k^* + G/2$ over the subspace of two occupied energy bands. The corresponding Wilson-loop eigenvalues are for the Wilson loop in the direction of the reciprocal lattice vector $G$ [67]. The signs $\pm$ represent $\pm 1$ if $\hat{Q}^2 = +1$ or $\pm i$ if $\hat{Q}^2 = -1$. c.c. stands for complex-conjugate pair of values of magnitude 1.

<table>
<thead>
<tr>
<th>$Q$ eigenval.</th>
<th>$Q$ eigenval.</th>
<th>Eigenval. of $W_{k^<em>+G-k^</em>}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(++)$</td>
<td>$(++)$</td>
<td>$(1,1)$</td>
</tr>
<tr>
<td>$(++)$</td>
<td>$(+-)$</td>
<td>$(1,-1)$</td>
</tr>
<tr>
<td>$(++)$</td>
<td>$(-)$</td>
<td>$(-1,-1)$</td>
</tr>
<tr>
<td>$(+-)$</td>
<td>$(+-)$</td>
<td>$(c.c.)$</td>
</tr>
</tbody>
</table>

In the degeneracy of the Wannier values at the TR-invariant momenta.

Additionally, the constraints due to the reflection $(M_x, M_y)$, inversion $(I)$ and $C_4$ symmetries are

\[
\begin{align*}
\{\nu_x^i(k_y)\} & \overset{M_x}{=} \{-\nu_x^i(k_y)\}, \\
\{\nu_y^i(k_y)\} & \overset{M_x}{=} \{\nu_y^i(-k_y)\}, \\
\{\nu_x^i(k_y)\} & \overset{I}{=} \{-\nu_x^i(-k_y)\}, \\
\{\nu_y^i(k_y)\} & \overset{C_4}{=} \{\nu_y^i(k_x = -k_y)\}, \\
\{\nu_y^i(k_x)\} & \overset{C_4}{=} \{-\nu_x^i(k_y = k_x)\}
\end{align*}
\]

(mod 1). Recall that in 2D inversion $I$ and $C_2$ transform the coordinates the same way, hence the constraints on the Wannier bands due to $C_2$ are the same as those generated by $I$ in 2D. Now, notice in particular that in the presence of the reflection symmetry $M_x$, the first relation implies that the Wannier bands are either flat bands locked to 0 or $\frac{1}{2}$, or can “disperse”, but must occur in pairs $\{-\nu_x(k_y), \nu_x(k_y)\}$. Since in gapped systems the values of $\nu_x^i(k_y)$ cannot change abruptly from 0 to $\frac{1}{2}$ across different values of $k_y \in [-\pi, \pi)$, $M_x$ reflection implies that the polarization is either $p_x = 0$ or $\frac{1}{2}$. This is the case in the insulators $h^1(k)$ and $h^2(k)$ with Hamiltonians (2.105), having Wannier bands as in Figs. 2.14(a) and 2.14(b). Notice that these descriptions are compatible with the constraints on the polarization in Eqs. (2.91) and (2.94). Indeed, in 2D, the constraints due to $M_x$ on $\nu_x(k_y)$ at each $k_y$ are the same as the constraints due to $I$ in 1D (see Eq 2.60). Thus, Table 2.2 in 1D is extended to Table 2.3 in 2D. These relations between inversion, reflection, and Wilson-loop eigenvalues can be verified in the insulators $h^1(k)$ and $h^2(k)$.
Wannier bands and the edge Hamiltonian

Being unitary, we can express the Wilson loop as the exponential of a Hermitian matrix,

\[ W_{C,k} \equiv e^{iH_{W_C}(k)}. \]  

We refer to \( H_{W_C}(k) \) as the \textit{Wannier Hamiltonian}. Notice that in the definition above, the argument \( k \) of the Wannier Hamiltonian is the base point of the Wilson loop. The eigenvalues of \( H_{W_C}(k) \) are precisely the Wannier bands, \( \{2\pi \nu_x(k_y)\} \) or \( \{2\pi \nu_y(k_x)\} \), which only depend on the coordinate of \( k \) normal to \( C \), e.g., in two-dimensions, the eigenvalues depend on \( k_y \) for \( C \) along \( k_x \) and vice versa.

The Wannier Hamiltonian \( H_{W_C}(k) \) has been shown to be adiabatically connected with the Hamiltonian at the edge perpendicular to \( C \) [66]. The map, however, is not an exact identification, but rather, one that preserves the topological properties of the Hamiltonian at the edge. The Wannier bands, being the spectrum of \( H_{W_C}(k) \), are adiabatically connected with the energy spectrum of the edge. Indeed, we see from Fig. 2.14 that this interpretation correctly describes the edge properties of the systems in Eq. (2.106). For example, we recognize the standard edge state patterns for the Chern insulator and the QSH insulator, while the weak topological insulator has a flat band of edge states as expected for an ideal system with vanishing correlation length.

Let us now mention some useful relations obeyed by the Wannier Hamiltonian. If we denote with \(-C\) the contour \( C \) but in reverse order, it follows that

\[ W_{-C,k} = W_{C,k}^\dagger = e^{-iH_{W_C}(k)}, \]  

thus, we make the identification

\[ H_{W_{-C}}(k) = -H_{W_C}(k). \]

Insulators with a lattice symmetry obey

\[ g_khkg_k^{-1} = h_{D_gk}, \]  

where \( g_k \) is the unitary operator \( g_k = e^{-i(D_gk)\cdot\delta}U_g \). Here, \( U_g \) is an \( N_{orb} \times N_{orb} \) matrix that acts on the internal degrees of freedom of the unit cell, and \( D_g \) is an operator in momentum space sending \( k \to D_gk \). In real space, on the other hand, we have \( r \to D_g r + \delta \), where \( \delta = 0 \) in the case of symmorphic symmetries,
or takes a fractional value (in unit-cell units) in the case of non-symmorphic symmetries.

Using the definition of the Wannier Hamiltonian (2.111), we can rewrite the expression for the transformation of Wilson loops [63] into the form

\[ B_{g,k}H_{Wc}(k)B_{g,k}^\dagger = H_{W_{Dg}c}(D_gk), \]  

where

\[ B_{g,k}^{mn} = \langle u^n_{Dgk} | g_k | u^m_k \rangle \]  

is the unitary sewing matrix that connects states at \( k \) with those at \( D_gk \) having the same energy.

Hence, we can interpret the usual sewing matrix \( B_{g,k} \) for the bulk Hamiltonian as a symmetry operator of the Wannier Hamiltonian. In particular, we have

\[ B_{M_x,k}H_{Wc}(k)B_{M_x,k}^\dagger = -H_{Wc}(M_xk), \]
\[ B_{M_y,k}H_{Wc}(k)B_{M_y,k}^\dagger = H_{Wc}(M_yk), \]
\[ B_{I,k}H_{Wc}(k)B_{I,k}^\dagger = -H_{Wc}(\pm k). \]  

### 2.5 Edge dipole moments in 2D crystals

Before discussing the bulk quadrupole moment in 2D insulators, we take the intermediate step of studying 2D crystalline insulators which may give rise to edge-localized polarizations [70]. In particular, we describe the procedure to calculate the position-dependent polarization in an insulator, and then we show in an example how the edge polarization arises. We start by considering a 2D crystal with \( N_x \times N_y \) sites. For calculating the polarization along \( x \) as a function of position along \( y \), we choose the insulator to have periodic boundary conditions along \( x \) and open boundary conditions along \( y \). In this configuration there is no crystal momenta \( k_y \), and we can treat this crystal as a wide, pseudo-1D lattice by absorbing the labels \( R_y \in 1 \ldots N_y \) into the internal degrees of freedom of an enlarged unit cell that extends along the entire length of the crystal in the \( y \)-direction. This is shown schematically in Fig. 2.15(b). Thus, the formulation in Sec. 2.3.2 follows through in this case, with the redefinition:

\[ c_{k,\alpha} \rightarrow c_{k_x, R_y, \alpha} \]  

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which allows us to write the second-quantized Hamiltonian as

$$H = \sum_{k_x} c_{k_x, R_y, \alpha}^{\dagger} [h_{k_x}]_{R_y, \alpha, R'_y, \beta} c_{k_x, R'_y, \beta},$$

(2.119)

for $\alpha, \beta \in 1 \ldots N_{\text{orb}}$, and $R_y, R'_y \in 1 \ldots N_y$. In the above redefinitions, notice that, since the boundaries remain closed along $x$, $k_x$ is still a good quantum number. We diagonalize this Bloch Hamiltonian as

$$[h_{k_x}]_{R_y, \alpha, R'_y, \beta} = \sum_n [u_{k_x}^n]_{R_y, \alpha} \epsilon_{n, k_x} [u_{k_x}^n]_{R'_y, \beta},$$

(2.120)

where $n \in 1 \ldots N_{\text{orb}}$. So, if the 2D Bloch Hamiltonian with periodic boundary conditions along $x$ and $y$, $h_{(k_x, k_y)}$, has $N_{\text{occ}}$ occupied bands, its associated pseudo-1D Bloch Hamiltonian $h_{k_x}$ in (2.120) has $N_{\text{occ}} \times R_y$ occupied bands. We can diagonalize the Hamiltonian (2.119) as

$$H = \sum_{n,k_x} \gamma_{n,k_x}^{\dagger} \gamma_{n,k_x},$$

(2.121)

where

$$\gamma_{n,k_x} = \sum_{R_y, \alpha} [u_{k_x}^n]_{R_y, \alpha} c_{k_x, R_y, \alpha}.$$

(2.122)

Following Sec. 2.3.2, the matrices

$$[G_{k_x}]^{mn} \equiv \sum_{R_y, \alpha} [u_{k_x}^m]_{R_y, \alpha} [u_{k_x}^n]_{R_y, \alpha},$$

(2.123)

are used in the construction of the Wilson line elements $[F_{k_x}]^{mn}$ (via singular value decomposition) and subsequently the Wilson loops $[W_{k_x + 2\pi \epsilon R_y}]^{mn}$, where $m, n \in 1 \ldots N_{\text{occ}} \times N_y$. Notice that the size of these Wilson-loop matrices is $N_y$-times larger than the size of Wilson-loop matrices when both boundaries are closed in the crystal.

The hybrid Wannier functions have the same form as in (2.45):

$$\left| \Psi_{R_x}^j \right> = \frac{1}{\sqrt{N_y}} \sum_{n=1}^{N_{\text{occ}}} \sum_{k_x} \left[ \nu_{k_x}^j \right]^n e^{-ik_x R_x \gamma_{n,k_x}} \left| 0 \right>,$$

(2.124)

for $j \in 1 \ldots N_{\text{occ}} \times N_y$, $R_x \in 1 \ldots N_x$, and where $\left[ \nu_{k_x}^j \right]^n$ is the $n$th component of the $j$th Wilson-loop eigenstate $\left| \nu_{k_x}^j \right>$, and $\gamma_{n,k_x}^{\dagger}$ is given in (2.122). In order to spatially resolve the $x$ component of the polarization
along the $y$ direction, we calculate the probability density of the hybrid Wannier functions (2.124),

$$
\rho^j_{R_x}(R_y) = \sum_{R_z,\alpha} \langle \Psi^j_{R_x} \mid \phi^{R_y,\alpha}_{R_z} \rangle \langle \phi^{R_y,\alpha}_{R_z} \mid \Psi^j_{R_x} \rangle
= \frac{1}{N_x} \sum_{k_x,\alpha} |(u^\alpha_{k_x})_{R_y,\alpha} [\nu^j_{k_x}]^n|^2
$$

(2.25)

(in the first equation above, no sums are implied over repeated indices). Notice that there is no dependence on the unit cell $R_x$, as expected since the density is translationally invariant in the $x$ direction. Thus, we can write $\rho^j_{R_x}$ simply as $\rho^j$. This probability density then allows us to resolve the hybrid Wannier functions (2.124) along the $y$-direction. In particular, it will let us determine whether any of these functions are localized at the (open) edges at $R_y = 0, N_y$. This probability density also allows us to calculate the $x$ component of the polarization via

$$
p_x(R_y) = \sum_j \rho^j(R_y) \nu^j_x
$$

(2.26)

which is resolved at each site $R_y$.

We now illustrate the existence of edge polarization with an example. Consider the insulator with Bloch Hamiltonian

$$
h(k) = \begin{pmatrix}
\delta \tau_0 & q(k) \\
q^\dagger(k) & -\delta \tau_0
\end{pmatrix},
q(k) = \begin{pmatrix}
\gamma + \lambda_x e^{i k_x} & \gamma + \lambda_y e^{i k_y} \\
\gamma + \lambda_y e^{-i k_y} & \gamma + \lambda_x e^{-i k_x}
\end{pmatrix},
$$

(2.27)

where $\tau_0$ is the $2 \times 2$ identity matrix, and $\tau_a$, $a = 1, 2, 3$, are Pauli matrices. A tight-binding representation of this model is shown in Fig. 2.15(a). $\gamma$ is the strength of the coupling within unit cells, represented by red lines in Fig. 2.15(a), and $\lambda_x$ and $\lambda_y$ are the strengths of horizontal and vertical hoppings between nearest-neighbor cells. $\delta$ is the amplitude of an on-site potential [Fig. 2.15(c)] that breaks reflection symmetry along $x$ and $y$, but maintains inversion symmetry. When $\delta = 0$, this model has reflection and inversion symmetries, with operators $\hat{M}_x = \tau_x \otimes \tau_0$, $\hat{M}_y = \tau_x \otimes \tau_x$, and $\hat{T} = \tau_0 \otimes \tau_x$.

This insulator also has fine-tuned chiral and time-reversal symmetries. However, since we are only interested in protection due to spatial symmetries, we add a small perturbation to (2.27) in our numerics of the form:

$$
h_{\text{pert}}(k) = EE \cos(k_x) + OE \sin(k_x) + EE \cos(k_y) + EO \sin(k_y),
$$

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Figure 2.15: Edge polarization in insulator with Hamiltonian (2.127) (inversion-symmetric). (a) Lattice with periodic boundaries. (b) Lattice with periodic boundaries along x and open along y. Long vertical rectangles are redefined unit cells in the pseudo-1D lattice construction. (c) On-site potential on the lattice. Red (blue) sites represent the on-site energies of +δ (−δ) that break $M_x$ and $M_y$ symmetry but preserve inversion. (d), (g) Wannier bands $\nu_x(k_y)$ and $\nu_y(k_x)$ for the configuration in (a) which has full periodic boundaries. (e) Wannier values $\nu_x$ and (f) polarization $p_x(R_y)$ for the configuration in (b) which has an open boundary. (h) Wannier values $\nu_y$ and (i) polarization $p_y(R_x)$ for a configuration as in (b) but with boundaries open along x and closed along y. In all plots we set $\lambda_x = 1$, $\lambda_y = 0.5$, $\gamma = 0.1$, $\delta = 0.2$, and the strength of the small perturbation to break chiral and time-reversal symmetries (see text) to 0.15. We verify that this perturbation does not close the energy gap.

where $EE$, $OE$, and $EO$ are $4 \times 4$ random matrices that obey

$$[EE, \hat{M}_x] = 0, \quad [EE, \hat{M}_y] = 0,$$

$$\{OE, \hat{M}_x\} = 0, \quad [OE, \hat{M}_y] = 0,$$

$$[EO, \hat{M}_x] = 0, \quad \{EO, \hat{M}_y\} = 0,$$

and with entries in the range $[0, 1]$. These nearest-neighbor perturbations break the chiral and time-reversal symmetries, while preserving the reflection symmetries along both $x$ and $y$, as well as inversion symmetry. These perturbations are added to ensure that the interesting features do not rely on these fine-tuned symmetries.
We first consider the general case of generating non-quantized edge polarizations by breaking reflection symmetries (Figs. 2.15 and 2.16), and later on discuss the special case in which these edge polarizations are quantized by restoring reflection symmetries (Fig. 2.17). In both cases, however, preserving inversion symmetry is necessary in order to have an overall vanishing bulk polarization. In particular, well-defined edge polarizations require that the edges do not accumulate charge and are neutral, hence, the bulk of the insulator should not be polarized.

For the general case of non-quantized edge polarizations, we consider $\lambda_x > \lambda_y$ and $\gamma \ll |\lambda_x - \lambda_y|$. Under these conditions, the crystal is an insulator at half-filling. The inversion eigenvalues of the occupied bands come in $\pm 1$ pairs at all symmetry points. Therefore, there is no protection of degeneracies in the Wannier bands, as we can see from the plots of $\nu_x(k_y)$ and $\nu_y(k_x)$ shown in Figs. 2.15(d) and 2.15(g). If all the boundaries of the system are closed, the crystal has uniform, vanishing bulk polarization protected by inversion symmetry. If instead we open the boundaries along $y$, as in Fig. 2.15(b), we can use the formulation from earlier in this section to treat this crystal as a pseudo-1D insulator, with redefined unit cells as shown by the long vertical rectangles in Fig. 2.15(b). The Wannier values $\nu_j^y$, for $j \in 1 \ldots 40$ ($N_{\text{occ}} = 2$, $N_y = 20$), obtained from this calculation are shown in Fig. 2.15(e). Using these values and their associated hybrid-Wannier functions, we calculate the polarization $p_y(R_x)$ using (2.126). This is shown in Fig. 2.15(f). Remarkably, although the polarization vanishes in the bulk, there is edge-localized polarization parallel to the edge. If, instead of opening the boundaries along $y$, we choose to open them in $x$, we observe the Wannier values $\nu_j^x$, for $j \in 1 \ldots 40$, and polarization $p_y(R_x)$ shown in Figs. 2.15(h) and 2.15(i), respectively. We find a vanishing polarization in the bulk, but non-zero edge-localized polarizations tangent to the edge. For our choice of $\lambda_x > \lambda_y$ the values of $|p_y|$ localized at the $R_x = 0, N_x$ edges are larger than the values $|p_x|$ localized at $R_y = 0, N_y$.

To complete the picture, we ask what happens if the edge polarization is terminated at a corner. Fig-
Figure 2.17: Insulator with Bloch Hamiltonian (2.127) and $\delta = 0$. Here, we set $\lambda_x > \lambda_y$. (a) $M_x$ eigenvalues along the $(0, k_y)$ and $(\pi, k_y)$. (b) $M_y$ eigenvalues along the $(k_x, 0)$ and $(k_x, \pi)$. (c) Wannier bands $\nu_x(k_y)$. (d) Wannier values $\nu_y$ when boundaries are open along $y$. (e) $p_x(R_y)$ for configuration as in (d). (f) Wannier bands $\nu_y(k_x)$. (g) Wannier values $\nu_y$ when boundaries are open along $x$. Values at $\nu_x = 0.5$ have edge localized eigenstates. (h) $p_y(R_x)$ for configuration as in (g). The parameters used here are as in Fig. 2.15 but with $\delta = 0$, except for (e) and (h), for which $\delta = 10^{-4}$.

Figure 2.16 shows the charge density in this insulator [Eq. (2.127)] when both boundaries are open. We see that, relative to the background charge density of $2e$ per unit cell, there are corner-localized charges $Q_{\text{corner}}$. These charges and the edge polarizations obey $Q_{\text{corner}} = p_{\text{edge}} x + p_{\text{edge}} y$, as expected for insulators with vanishing bulk dipole and quadrupole moments (Sec. 2.2.4). As such, this polarization is purely a surface effect [70] and not generated by a bulk quadrupole moment.

Now let us consider the case with reflection symmetry. As is typical for these types of calculations we still must break the reflection symmetries infinitesimally by setting $0 < \delta \ll \gamma, \lambda_x, \lambda_y$. This infinitesimal, non-zero $\delta$ perturbation breaks reflection symmetries softly and is necessary to choose an unambiguous sign for the quantized edge polarizations. In a lattice with full open boundary conditions, this perturbation serves to split the degeneracy of the four corner-localized mid-gap modes to determine how they are filled at half-filling. This then chooses the signs of the corner charges in a way consistent with the choice of edge polarizations.

We find that for $\lambda_x > \lambda_y$ we have $Q_{\text{corner}} = p_{\text{edge}} y = \frac{1}{2}$ and $p_{\text{edge}} x = 0$, while for $\lambda_y > \lambda_x$ we find
$Q_{\text{corner}} = p_{\text{edge}}x = \frac{1}{2}$ and $p_{\text{edge}}y = 0$. Let us focus on the case $\lambda_x > \lambda_y$. By setting $\delta = 0$, the reflection eigenvalues for this insulator are indicated in Figs. 2.17(a) and 2.17(b). Based on the analysis of reflection eigenvalues summarized in Table 2.3, we conclude that $M_x$ fixes the Wannier bands to $\nu_{x,1}^{1,2}(k_y) = \frac{1}{2}$, as in Fig. 2.17(c), while $M_y$ does not restrict the values of $\nu_{y}^{1,2}(k_x)$ to either 0 or $\frac{1}{2}$. Instead, they only have to obey $\nu_{y}^{1}(k_x) = -\nu_{y}^{2}(k_x)$, as in Fig. 2.17(f). If we now open the boundaries along $y$ and calculate $\nu_{y}^{j}$, we obtain degenerate values $\nu_{y}^{j} = \frac{1}{2}$ [Fig. 2.17(d)], which result in $p_{y}(R_y) = 0$ [Fig. 2.17(e)]. If we instead open the boundaries along $x$ and calculate $\nu_{x}^{j}$ we obtain the gapped bands which have corresponding Wannier eigenstates that have weight primarily in the bulk of the sample. Interestingly, in addition to the gapped bulk Wannier states, we find a pair of Wannier values pinned at $\frac{1}{2}$ that have eigenstates localized at the edges $R_x = 0$ and $N_x$ [Fig. 2.17(g)]. It is this pair of states that results in the edge polarization of $\pm \frac{1}{2}$, as shown in Fig. 2.17(h) (a small value of $\delta = 10^{-4}$ was chosen for plots e and h to break Wannier degeneracies).

In contrast to this phenomenology, we will see in Sec. 2.6 that insulators with quadrupole moments also have edge-localized polarizations and corner-localized charges, but, unlike in the present case, these boundary properties obey $|Q_{\text{corner}}| = |p_{\text{edge}}x| = |p_{\text{edge}}y|$, as required for a quadrupole (see Sec. 2.2.4).

### 2.6 Bulk quadrupole moment in 2D crystals

Any quadrupole insulator should have three basic properties: (i) its bulk dipole moment must vanish, otherwise the quadrupole moment is ill-defined (see Sec. 2.2.2); (ii) the insulator must have at least two occupied bands, since a crystal with one occupied band can only generate dipole moments (a quadrupole is made from two separated dipoles); and (iii) it should have edges that are insulators themselves, as only insulating edges can host edge-localized polarization (hence, edges should not host gapless states and thus the bulk must have Chern number $n = 0$).

From the classical analysis of Sec. 2.2.3 we concluded that the boundary signatures of an ideal 3D insulator with only bulk quadrupole moment density are the existence of charge density per unit length at hinges $\lambda_{\text{hinge}}^{a,b} = \frac{1}{2} n_{i}^{(a)} n_{j}^{(b)} q_{ij}$ and polarization density per unit area at faces $p_{\text{face}}^{a} = n_{i}^{(a)} q_{ij}$, where in these two expressions summation is implied over repeated indices. In 2D, these expressions reduce to corner charges and edge polarization density per unit length, respectively:

$$Q_{\text{corner}}^{a,b} = \frac{1}{2} n_{i}^{(a)} n_{j}^{(b)} q_{ij}, \quad p_{\text{edge}}^{a} = n_{i}^{(a)} q_{ij},$$

(2.128)

In the expressions above, $q_{ij}$ is the quadrupole moment per unit area, with $q_{xy} = q_{yx} \neq 0$, $q_{xx} = q_{yy} = 0$.

The insulator with Hamiltonian (2.127) meets all the three basic requirements: it is an insulator with
two electrons per unit cell, zero bulk polarization, and no Chern number. Furthermore, it does have corner charges when both boundaries are open. However, it fails to meet the relations (2.128); its edge polarizations are not of the same magnitude as its corner charge. Instead, they obey $Q_{\text{corner}} = p_{\text{edge}}^x + p_{\text{edge}}^y$ (see Sec. 2.5) and can be accounted for by the theory of polarization up to dipole moments (see Sec. 2.2.4).

In this section, we describe a model realization of a symmetry-protected quadrupole insulator, an insulator with vanishing dipole moment and fractional, quantized quadrupole moment, that manifests through the predicted boundary signatures of Eq. (2.128). This model has two occupied bands and a vanishing Chern number. Crucially, its pair of Wannier bands are gapped, and each Wannier band can have an associated Berry phase. Physically, this corresponds to a bulk configuration in which two parallel dipoles aligned along one direction are separated along its perpendicular direction. We first describe the formalism of Wannier band topology for 2D insulators and then describe the observables of a quadrupole insulator. We will then explore the quantization of dipole pumping resulting from nontrivial adiabatic cycles that connect the quadrupole and trivial phases, and end with a description of an insulator with hinge-localized chiral modes in 3D which exhibits the same topology as the dipole pumping process.

### 2.6.1 Wannier-sector polarization

In this section, we study the topology of Wannier bands $\nu_x(k_y)$ that are gapped across the entire 1D BZ $k_y \in (-\pi, \pi]$, a minimal example of which is shown in Fig. 2.18. Due to the gap in the Wannier spectrum around $\nu_x = \frac{1}{2}$ we can broadly define two Wannier sectors

\[
\nu_x^- = \{ \nu_x^j(k_y), \text{ s.t. } \nu_x^j(k_y) \text{ is below the Wannier gap} \}
\]

\[
\nu_x^+ = \{ \nu_x^j(k_y), \text{ s.t. } \nu_x^j(k_y) \text{ is above the Wannier gap} \}.
\]

Since the Wannier bands are defined mod 1, we adopt the convention of defining the Wannier sectors $\nu_x^- \in [0, \frac{1}{2})$ and $\nu_x^+ \in [\frac{1}{2}, 1)$.

We then choose those above or below the gap and form the projector

\[
P_{\nu_x} = \sum_{j=1}^{N_W} \sum_{R_x,k_y} \left| \Psi_j^{R_x,k_y} \right\rangle \left\langle \Psi_j^{R_x,k_y} \right| = \sum_{j=1}^{N_W} \sum_{n,m=1}^{N_{\text{occ}}} \sum_k \gamma_n^{\dagger} \left| 0 \right\rangle \left| \nu_x^j,n \right\rangle \left\langle \nu_x^j,m \right| \left\langle 0 \right| \gamma_m \left(2.129\right)
\]

where $\sum_i^{N_W}$ is a summation over all Wannier bands in the sector $\nu_x$, for $\nu_x = \nu_x^+$ or $\nu_x^-$. $N_W$ is the number
Figure 2.18: Gapped Wannier bands $\nu^\pm_x(k_y)$ (red lines to the right of the BZ) and $\nu^\pm_y(k_x)$ (blue lines above of the BZ) of the quadrupole insulator with Hamiltonian (2.156).

of Wannier bands in sector $\nu_x$. $R_x \in 0 \ldots N_x - 1$ labels the unit cells, $k_y = \Delta k_y n_y$, for $\Delta k_y = 2\pi/N_y$, and $n_y \in 0, 1, \ldots, N_y - 1$ is the crystal momentum along $y$.

We are interested in studying the topological properties of the subspace spanned by $P_{\nu_x}$. As we will see in Sec. 2.4.2, the topology of the Wannier sectors is related to the topology of the physical edge Hamiltonian. As such, it will provide a bulk measure of the edge topology. In particular, we want to diagonalize the position operator,

$$\hat{y} = \sum_{R,\alpha} \hat{c}_{R,\alpha}^\dagger |0\rangle e^{-i\Delta k_y (R_y + r_{\alpha,y})} \langle 0| \hat{c}_{R,\alpha}$$

$$= \sum_{k_x,k_y,\alpha} \hat{c}_{k_x,k_y,\alpha}^\dagger |0\rangle \langle 0| c_{k_x,k_y,\alpha},$$

(2.130)

projected into the Wannier sector $\nu_x$,

$$P_{\nu_x} \hat{y} P_{\nu_x} = \sum_{j,j'=1}^{N_W} \sum_{k} \sum_{n,m,n',m'=1}^{N_{occ}} \gamma_{n,k+\Delta k_y}^m |0\rangle \langle 0| \gamma_{n',k}^{m'}$$

$$\times \left( \nu^{j}_{j',k+\Delta k_y} |\nu^{j}_{j',k+\Delta k_y}\rangle \nu^{m}_{m',k+\Delta k_y} |\nu^{m'}_{m',k}\rangle \nu^{m'}_{m',k} |\nu^{m'}_{m',k}\rangle \nu^{j'}_{j',k} |\nu^{j'}_{j',k}\rangle \nu^{j'}_{j',k} |\nu^{j'}_{j',k}\rangle \right).$$

(2.131)

To simplify the notation let us define the Wannier band basis

$$|w_{j,\alpha}\rangle = \sum_{n=1}^{N_{occ}} \nu^n_{j,k} |\nu^{j}_{j,k}\rangle \nu^{j}_{m',k} |\nu^{j'}_{j',k}\rangle$$

(2.132)
for \( j \in 1 \ldots N_W \). This basis obeys,

\[
\langle w_{x,k}^j | w_{x,k}^{j'} \rangle = \delta_{j,j'}.
\] (2.133)

However, in general, \( \langle w_{x,k}^j | w_{x,q}^{j'} \rangle \neq \delta_{j,j'} \delta_{k,q} \). The projected position operator then reduces to

\[
P_{\nu_x} \hat{y} P_{\nu_x} = \sum_{j,j' = 1}^{N_W} \sum_{k} \sum_{n,n'} \gamma_n^{\dagger} \gamma_n |0\rangle \langle 0 | \gamma_n',k \times \left( \langle \nu_x^j | \nu_x^{j'} \rangle \right) |\nu_x^j, \nu_x^{j'}, k \rangle.
\] (2.134)

Notice that the operator is diagonal in \( k_z \). Explicitly,

\[
P_{\nu_x} \hat{y} P_{\nu_x} = \sum_{k_x, k_y} \sum_{n,n'} \gamma_n^{\dagger} \gamma_n |0\rangle \langle 0 | \gamma_n', k_{x,y} \times \left( \langle \nu_x^j | \nu_x^{j'} \rangle \right) |\nu_x^j, \nu_x^{j'}, k_{x,y} \rangle.
\] (2.135)

where

\[
[F_{\nu_x}^{\nu_y(k_x,k_y)}]^{n,n'} = \sum_{j,j'=1}^{N_W} \left( \langle \nu_x^j | \nu_x^{j'} \rangle \right) |\nu_x^j, \nu_x^{j'}, k_{x,y} \rangle.
\] (2.136)

To diagonalize \( P_{\nu_x} \hat{y} P_{\nu_x} \), we calculate the Wilson loop along \( y \):

\[
|W_{\nu_x}^{\nu_y} \rangle^{n,n'} = F_{\nu_x,k + \Delta_{k_y}} \cdots F_{\nu_y,k_{x,y} + \Delta_{k_y}} F_{\nu_y,k}
\]

\[
= \left( \langle \nu_x^j | \nu_x^{j'} \rangle \right) \left( |W_{\nu_x}^{\nu_y} \rangle \right)^{n,n'}
\]

\[
= \left( \langle \nu_x^j | \nu_x^{j'} \rangle \right) \left( |W_{\nu_x}^{\nu_y} \rangle \right)^{n,n'}.
\] (2.137)

for \( n,n' \in 1 \ldots N_{\text{occ}} \), and \( j,j' \in 1 \ldots N_W \). \( W_{\nu_x}^{\nu_y} \) is the Wilson loop along \( y \) over the Wannier sector \( \nu_x \) performed over the Wannier band basis,

\[
|W_{\nu_x}^{\nu_y} \rangle^{j,j'} = \left( \langle w_{x,k + \Delta_{k_y}}^{r} | w_{x,k + (N_y - 1)\Delta_{k_y}}^{r} \right) \cdots \left( \langle w_{x,k + \Delta_{k_y}}^{s} | w_{x,k}^{s} \right) \cdots \left( \langle w_{x,k + (N_y - 1)\Delta_{k_y}}^{s} | w_{x,k}^{s} \right).
\] (2.138)

In the expression above, summation is implied over repeated indices \( r, \ldots, s \in 1 \ldots N_W \) over all Wannier bands in the Wannier sector \( \nu_x \).

Since \( N_W < N_{\text{occ}} \), this Wilson loop (2.138) is calculated over a subspace within the subspace of occupied energy bands. In general, we will indicate an operator written in a Wannier band basis with a tilde, while no tilde indicates that it is written in the basis of energy bands. Since we have used \( \nu_x \) as the label for the
Wannier bands along $x$, we will use the labels $\nu_y^{\nu_x}$ for the eigenvalues and eigenvectors of the Wilson loop along $y$ carried out for the Wannier band sector $\nu_x$. This Wilson loop diagonalizes as

$$\tilde{W}_{y,k,\nu_x} | \nu_y^{\nu_x,j} \rangle = e^{i 2\pi \nu_y^{\nu_x,j}(k_x)} | \nu_y^{\nu_x,j} \rangle$$

(2.139)

for $j \in 1 \ldots N_W$. The polarization over the Wannier sector $\nu_x$ at $k_x$ is then given by the sum of the $N_W$ phases $\nu_y^{\nu_x}(k_x)$:

$$p_y^{\nu_x}(k_x) = \sum_{j=1}^{N_W} \nu_y^{\nu_x,j}(k_x) \text{ mod } 1.$$ 

(2.140)

This can be written as

$$p_y^{\nu_x}(k_x) = -\frac{i}{2\pi} \text{Log Det}[\tilde{W}_{y,k,\nu_x}].$$

(2.141)

The total polarization of the Wannier bands $\nu_x$ is

$$p_y^{\nu_x} = \frac{1}{N_x} \sum_{k_x} p_y^{\nu_x}(k_x).$$

(2.142)

In the thermodynamic limit it becomes

$$p_y^{\nu_x} = -\frac{1}{(2\pi)^2} \int_{BZ} \text{Tr}[\tilde{A}^\nu_{y,k}] d^2k$$

(2.143)

where $\tilde{A}_{y,k}^{\nu_x}$ is the Berry connection of Wannier bands $\nu_x$ having components

$$[\tilde{A}^\nu_{y,k}]_{j,j'} = -i \left< w_{x,k}^j | \partial_{k_y} | w_{x,k}^{j'} \right>,$$

(2.144)

where $j,j' \in 1 \ldots N_W$ run over the Wannier bands in Wannier sector $\nu_x$.

The Wannier-sector polarization has a physical significance. In the bulk of the material, a Wannier gap for the Wilson loop along $x$ implies the existence of a spatial separation between electrons along $x$. For example, for the Wannier bands of Fig. 2.18, electrons in the sector $\nu_x^-$ are on the left side of the unit cell, and those in sector $\nu_x^+$ are on its right side. Thus, a non-zero polarization in the $y$-direction of such a Wannier sector represents a translation, up or down, of the electrons of that sector.

We can see a simple example of this for the insulator $h^1(k)$ [Eq. (2.105)]. Since its Wannier bands are flat, we can assign the values $\{\nu_x^-, \nu_x^+\} = \{0, \frac{1}{2}\}$ [see Fig. 2.14(a)]. The polarization along $y$ of each of these
Wannier bands gives the centers \( \{ \nu_y^{\nu^-}, \nu_y^{\nu^+} \} = \{ \frac{1}{2}, 0 \} \). Thus, the electron in the middle of the unit cell along \( x \) is in-between unit cells along \( y \), and vice versa [see Fig. 2.12(a)]. For this model, the position operators along \( x \) and \( y \) projected into the full subspace of occupied bands commute, and this insulator has the 2D Wannier representation shown in Fig. 2.12(a). The concept illustrated here, however, is also valid in cases in which the projected position operators along different directions do not commute, as long as the Wannier bands are gapped. This happens in the model that realizes a topological quadrupole insulator with the Wilson-loop structure shown in Fig. 2.19. The solid half-circles represent the maximally localized Wannier centers of the electrons in a minimal quadrupole insulator, to be described in detail in Sec. 2.6.4.

Consider Fig. 2.19. If we first diagonalize the Wilson loop along \( x \) at each \( k_y \), we find two Wannier bands, \( \nu_x^{\pm}(k_y) \), separated by a gap. Since these Wannier bands depend on the value of \( k_y \), this is not an extremely sharp resolution of the position of the electronic charge along \( x \). However, the existence of the Wannier gap implies that there are two clouds of electrons, one corresponding to each Wannier sector: one to the right of the middle of the unit cell and another one to its left (the center of the unit cell is at the center of each panel). Thus, we can assign an average \( x \) coordinate to each cloud by calculating the average values of the Wannier bands, i.e., \( \nu_x^{\pm} = \frac{1}{N_y} \sum_{k_y} \nu_x^{\pm}(k_y) \). Furthermore, we can resolve the position of each of these two electronic clouds along \( y \) by calculating the nested Wilson loop (2.138). This yields \( p_y^{\nu^+} = p_y^{\nu^-} = \frac{1}{2} \) in the non trivial quadrupole phase, as in Fig. 2.19, or \( p_y^{\nu^+} = p_y^{\nu^-} = 0 \) in the trivial phase (not shown). In Fig. 2.19 we also show the localization if we first resolve the electronic positions along \( y \) and then along \( x \). The electronic localizations thus depend on the order in which the positions along \( x \) and \( y \) are resolved. This is a testament to the fact that the projected position operators along \( x \) and \( y \) do not commute.

Notice that, in the two paths for electron localization represented in Fig. 2.19, the overall bulk polarization vanishes, which is a requirement for a well-defined quadrupole moment (see Sec. 2.2.2). Since the overall polarization in the bulk has contributions from both Wannier sectors, it follows that

\[
p_y^{\nu^+} + p_y^{\nu^-} = 0 \mod 1
\]

for a well-defined quadrupole moment. This can be enforced by inversion symmetry.
Figure 2.19: Wannier centers within the unit cell of a quadrupole insulator in the non trivial phase [see Hamiltonian (2.156) for the minimal quadrupole insulator] upon calculation of the Wilson loop \( W_y, k \) followed by \( W_{\nu x}, k \) (blue path) or \( W_{\nu y}, k \) (red path). The overall localizations do not coincide for these two paths because \( [P_{occ} \tilde{P}_{occ}, P_{occ} \tilde{P}_{occ}] \neq 0 \). The quadrupole insulator has two electrons per unit cell.

2.6.2 Symmetry protection and quantization of the Wannier-sector polarization

Under reflections \( M_x, M_y \), and inversion \( I \) the Wannier-sector polarizations obey

\[
\begin{align*}
\nu^\pm_y M_x &= \nu^\mp_y, \\
\nu^\pm_y M_y &= -\nu^\pm_y \implies \nu^\pm_y M_y &= 0 \text{ or } \frac{1}{2}, \\
\nu^\pm_y I &= -\nu^\mp_y
\end{align*}
\]

mod 1. The relations for \( \nu^\pm_x \) are the same as the above with the exchange of labels \( x \leftrightarrow y \). In 2D, the constraints generated by \( C_2 \) symmetry are the same as those generated by inversion symmetry \( I \).

In the expressions (2.146), \( M_y \) directly quantizes \( \nu^\pm_y \), \( M_x \), on the other hand, also requires \( I \) to quantize \( \nu^\pm_y \) [see first and third relations in Eq. (2.146)]. Since in spinless systems the existence of both reflection symmetries implies the existence of inversion symmetry, the Wannier-sector polarizations \( \nu^\pm_y \) and \( \nu^\pm_x \) (calculated from \( W_{\nu y, k} \) and \( W_{\nu x, k} \), respectively) of a system with both reflection symmetries take quantized
values

\[ p^\pm_y, p^\pm_x M_x, M_y \equiv 0 \text{ or } \frac{1}{2}. \]  

(2.147)

The quantization due to reflection symmetries can be used to compute the Wannier-sector polarization in a simpler way. The Wannier band basis (2.132) obeys

\[ \hat{M}_y \left| w^\pm_{x,(k_x,k_y)} \right\rangle = \alpha^\pm_{M_y} (k_x,k_y) \left| w^\pm_{x,(k_x,-k_y)} \right\rangle \]  

(2.148)

with a \( U(1) \) phase \( \alpha^\pm_{M_y} (k_x,k_y) \). In particular, at the reflection-invariant momenta, \( k_{xy} = 0 \) and \( \pi \), \( \alpha^\pm_{M_y} (k_x,k_{xy}) \) are the eigenvalues of the reflection representation of \( \left| w^\pm_{x,k} \right\rangle \) at \( (k_x,k_{xy}) \). These can take the values \( \pm 1 \) (\( \pm i \)) for spinless (spinfull) fermions. If the representation is the same (different) at \( k_{xy} = 0 \) and \( k_{xy} = \pi \), the Wannier-sector polarization is trivial (nontrivial) [18]. Thus, in reflection-symmetric insulators the Wannier-sector polarization can then be computed by

\[ \exp \left\{ i 2\pi p^\pm_y \right\} = \alpha^\pm_{M_y} (k_x,0) \alpha^\mp*_{M_y} (k_x,\pi), \]  

(2.149)

where the asterisk stands for complex-conjugation. The Wannier-sector polarization then takes the quantized values

\[ p^\pm_y M_y \equiv \begin{cases} 0, & \text{if trivial} \\ \frac{1}{2}, & \text{if nontrivial.} \end{cases} \]

### 2.6.3 Conditions for the existence of a Wannier gap

In the previous subsection, we saw that reflection symmetries quantize the Wannier-sector polarization. This Wannier-sector polarization is well defined only if the Wannier bands are gapped. In this section, we show that, in order to have gapped Wannier bands in the presence of reflection symmetries, \( M_x \) and \( M_y \), the reflection operators must not commute. We will prove this by showing that if the reflection operators commute, we necessarily have gapless Wannier bands [63], i.e.,

\[ [\hat{M}_x, \hat{M}_y] = 0 \implies \text{gapless Wannier bands}. \]  

(2.150)
Two natural ways to have noncommuting reflection symmetries are to have a model with a magnetic flux so that reflection is only preserved up to a gauge transformation, or to have spin-$\frac{1}{2}$ degrees of freedom. For our quadrupole model below we chose the former interpretation for the simplicity of the description.

For a crystal with $N_{\text{occ}}$ occupied energy bands and reflection and inversion symmetries $M_x$, $M_y$, and $I$, such that $[\hat{M}_x, \hat{M}_y] = 0$, various cases need to be considered [63]:

- $N_{\text{occ}} = 2$: In this case, the Wannier bands $\nu_x(k_y)$ are necessarily gapless at $k_y = 0, \pi$.
- $N_{\text{occ}} = 4$: In this case, the Wannier bands $\nu_x(k_y)$ can be generically gapped, with each Wannier sector being two-dimensional. The two eigenvalues of the nested Wilson loop over the Wannier sector $\nu_x$, for either $\nu_x = \nu_x^+$ or $\nu_x^-$ can be shown to come in pairs ($\nu_y^{\nu_x}(k_x), -\nu_y^{\nu_x}(k_x)$) at $k_x = 0, \pi$. This implies that $p_{\nu_y} = 0$.
- $N_{\text{occ}} = 4n$: In this case, we have a generalized version of the $N_{\text{occ}} = 4$ case.
- $N_{\text{occ}} = 4n + 2$: In this case, the Wannier bands split as in the $4n$ case plus a leftover set of two bands, and the Wannier spectrum is gapless.
- $N_{\text{occ}}$ is odd: In this case, the Wannier bands split as in one of the even band cases above plus one extra band. The extra band is always gapless, as its value is necessarily 0 or $\frac{1}{2}$ since it does not have partner (see Sec. 2.3.4).

Here we will elaborate on the first case. The other cases for generic numbers of bands are detailed in Ref [63]. Consider a spinless crystal with reflection symmetries $M_x$ and $M_y$. For a tight-binding Hamiltonian $h(k_x, k_y)$, these symmetries are expressed by Eq. (2.89). Such a system also has the inversion symmetry expressed by Eq. (2.95). The reflection operators $\hat{M}_{x,y}$ and the inversion operator $\hat{I}$ are related by

$$\hat{I} = \hat{M}_y \hat{M}_x.$$ \hspace{1cm} (2.151)

We should be careful at this point to note that in some 2D systems this definition of inversion is problematic since the operator $\hat{I}$ should obey $\hat{I}^2 = 1$. If we have $\hat{M}_y \hat{M}_x = -\hat{M}_y \hat{M}_x$, as we will encounter later, then by this definition $\hat{I}^2 = -1$ and so we should more precisely identify $\hat{M}_y \hat{M}_x$ as a $C_2$ rotation operator in 2D instead.

The special high-symmetry points and lines in the Brillouin zone, at which a given operator $\hat{Q}$ (we consider $\hat{Q} = \hat{M}_x, \hat{M}_y$ and $\hat{I}$) commutes with the Hamiltonian,

$$[h_{k_x}, \hat{Q}] = 0,$$ \hspace{1cm} (2.152)
Table 2.4: States with eigenvalues (+−) for $M_x$ and $M_y$ and their $\mathcal{I}$ eigenvalues at the high-symmetry points. The signs ± represent ±1 if $\hat{M}_{x,y}^2 = +1$ or ±i if $\hat{M}_{x,y}^2 = −1$. Also, $s = 0$ ($s = 1$) if $M_{x,y} = +1$ ($M_{x,y} = −1$).

<table>
<thead>
<tr>
<th>states</th>
<th>$M_x$ eigenval.</th>
<th>$M_y$ eigenval.</th>
<th>$\mathcal{I}$ eigenval.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(</td>
<td>++\rangle,</td>
<td>−−\rangle)$</td>
<td>(+−)</td>
</tr>
<tr>
<td>$(</td>
<td>−−\rangle,</td>
<td>++\rangle)$</td>
<td>(+−)</td>
</tr>
</tbody>
</table>

are shown in Fig. 2.10 in blue for $M_x$, red for $M_y$, and black dots for all $M_x$, $M_y$, and $\mathcal{I}$. We are interested in the conditions under which we have gapped Wannier bands along both $x$ and $y$. This can be inferred from the $\hat{Q}$ eigenvalues at the high-symmetry points [67], as shown in Table 2.3.

There we see that, in order to have gapped Wannier bands, the Wilson-loop eigenvalues must come in complex conjugate pairs $\{\xi, \xi^*\}$ not pinned at 1 or −1. Hence, we require that, along each of the blue and red lines of Fig. 2.10, the reflection eigenvalues come in pairs (+−). To these two conditions (one along blue lines for $\hat{M}_x$ eigenvalues and another one along red lines for $\hat{M}_y$ eigenvalues) we need to add the third requirement that the inversion eigenvalues must also come in pairs (+−) at the high-symmetry points $k^* = \Gamma, X, Y, M$ of the BZ. If the condition is not also met for the inversion eigenvalues, the complex conjugate pairs are still forced to be a pair of 1 or pair of −1 at $k_y = 0, \pi$ for Wilson loops along $k_x$, and at $k_x = 0, \pi$ for Wilson loops along $k_y$. We will now see that this third condition is not possible to meet simultaneously with the first two conditions if the reflection operators commute. If we have

$$[\hat{M}_x, \hat{M}_y] = 0,$$

it is possible to simultaneously label the energy states at the high-symmetry points by their reflection eigenvalues, e.g., $|m_x, m_y\rangle$, where

$$\hat{M}_x |m_x, m_y\rangle = m_x |m_x, m_y\rangle, \quad \hat{M}_y |m_x, m_y\rangle = m_y |m_x, m_y\rangle,$$

(2.153)

for reflection eigenvalues $m_{x,y} = \pm$. Since the inversion operator is $\hat{\mathcal{I}} = \hat{M}_x \hat{M}_y = \hat{M}_y \hat{M}_x$, the inversion eigenvalues are

$$\hat{\mathcal{I}} |m_x, m_y\rangle = m_x m_y |m_x, m_y\rangle.$$

(2.154)

The two combinations of states that have $\hat{M}_x$ and $\hat{M}_y$ eigenvalues of (+−) are listed in Table 2.4. However, those two options do not meet the third condition of having $\hat{\mathcal{I}}$ eigenvalues (+−) at the high-symmetry points. Instead, the $\hat{\mathcal{I}}$ eigenvalues at the high-symmetry points are always either (++) or (−−). These
inversion eigenvalues imply that the Wilson-loop eigenvalues come in complex conjugate pairs \( \{ \xi, \xi^* \} \), with \( \xi = \xi^* = +1 \) or \( -1 \). Thus, along the high-symmetry lines (blue and red lines of Fig. 2.10) the Wilson loops have eigenvalues

\[
\{ \xi, \xi^* \} \rightarrow \{ 1, 1 \} \text{ or } \{ -1, -1 \},
\]

i.e., at those lines the Wannier bands close the gap. Conversely, if instead of imposing the conditions of having \((+−)\) for both \( \hat{M}_x \) and \( \hat{M}_y \) eigenvalues, we started by first fixing \((+−)\) for \( \hat{I} \) eigenvalues, at most only one of the reflection eigenvalues will be \((+−)\). The other one will necessarily have either \((++\) or \((-−)\). An example of this case is insulator (2.127) with \( \delta = 0 \), with reflection eigenvalues shown in Figs. 2.17(a) and 2.17(b).

### 2.6.4 Simple model with topological quadrupole moment

We now focus on the detailed description of a model for an insulator with a quadrupole moment. The minimal model is a 2D crystal with two occupied bands. For simplicity we choose a microscopic representation consisting of four spinless fermion orbitals with Hamiltonian

\[
H^q = \sum_{\mathbf{R}} \left[ \gamma_x \left( c_{\mathbf{R},1}^\dagger c_{\mathbf{R},3} + c_{\mathbf{R},2}^\dagger c_{\mathbf{R},4} + \text{H.c.} \right) + \gamma_y \left( -c_{\mathbf{R},1}^\dagger c_{\mathbf{R},4} + c_{\mathbf{R},2}^\dagger c_{\mathbf{R},3} + \text{H.c.} \right) \\
+ \lambda_x \left( c_{\mathbf{R},1}^\dagger c_{\mathbf{R}+\hat{x},3} + c_{\mathbf{R},4}^\dagger c_{\mathbf{R}+\hat{x},2} + \text{H.c.} \right) + \lambda_y \left( -c_{\mathbf{R},1}^\dagger c_{\mathbf{R}+\hat{y},4} + c_{\mathbf{R},3}^\dagger c_{\mathbf{R}+\hat{y},2} + \text{H.c.} \right) \right],
\]

(2.155)

where \( c_{\mathbf{R},i}^\dagger \) is the creation operator for degree of freedom \( i \) in unit cell \( \mathbf{R} \), for \( i = 1, 2, 3, 4 \) as shown in Fig. 2.20(a). \( \gamma_x \) and \( \gamma_y \) represent amplitudes of hopping within a unit cell. \( \lambda_x \) and \( \lambda_y \) represent the amplitudes of hopping to nearest-neighbor unit cells along \( x \) and \( y \), respectively. The negative signs, represented by the dashed lines in Fig. 2.20(a), are a gauge choice for the \( \pi \) flux threaded through each plaquette (including within the unit cell itself). The corresponding Bloch Hamiltonian is

\[
h^q(\mathbf{k}) = [\gamma_x + \lambda_x \cos(k_x)] \Gamma_4 + \lambda_x \sin(k_x) \Gamma_3 + [\gamma_y + \lambda_y \cos(k_y)] \Gamma_2 + \lambda_y \sin(k_y) \Gamma_1,
\]

(2.156)

where \( \Gamma_0 = \tau_3 \otimes \tau_0 \), \( \Gamma_k = -\tau_2 \otimes \tau_k \), \( \Gamma_4 = \tau_1 \otimes \tau_0 \) for \( k = 1, 2, 3 \), where \( \tau_{1,2,3} \) are Pauli matrices, and \( \tau_0 \) is the \( 2 \times 2 \) identity matrix. The energy bands are

\[
\epsilon(\mathbf{k}) = \pm \sqrt{\epsilon_x^2(k_x) + \epsilon_y^2(k_y)}
\]

(2.157)
Figure 2.20: Minimal model with quadrupole moment having the Bloch Hamiltonian Eq. (2.156). (a) Lattice and (b) energy spectrum. Dashed lines in (a) have a negative sign to account for a flux of $\pi$ threading each plaquette. In (b) each energy band is twofold degenerate.

where $\epsilon_i(k_i) = \sqrt{\gamma_i^2 + 2\gamma_i\lambda_i \cos(k_i)} + \lambda_i^2$ for $i = x, y$. Each of the upper and lower energy bands is twofold degenerate.

This Hamiltonian is gapped across the entire bulk Brillouin zone (BZ) unless $|\gamma_x/\lambda_x| = 1$ and $|\gamma_y/\lambda_y| = \pm 1$. A plot of the energy spectrum in the 2D BZ is shown in Fig. 2.20(b) for $\gamma_x/\lambda_x = \gamma_y/\lambda_y = 0.5$. We consider this system at half-filling so that only the lowest two bands are occupied. This Hamiltonian has vanishing polarization, and zero Chern number for the entire range of parameters for which it is gapped. Thus, it meets the preliminary requirements of an insulator with quadrupole moment density outlined at the beginning of Sec. 2.6. The projected position operators along $x$ and $y$ do not commute at half-filling, and the Hamiltonian has a pair of gapped Wannier bands, as shown in Fig. 2.18.

In the present form, this Hamiltonian has symmetries that quantize the Wannier-sector polarizations $p_y^\pm, p_x^\pm = 0$ or $\frac{1}{2}$, which we describe in the following subsection. Associated to this quantization is the existence of sharply quantized corner charges and edge polarizations, in agreement with (2.128). Upon breaking the symmetries that quantize the quadrupole moment, a generalized version of this model can generate values of quadrupole moment satisfying $q_{xy} \in (0, 1]$. As an extension, we will see that when coupling this system to an adiabatically varying parameter, a quantum of dipole can be pumped in a way analogous to the quantum of charge pumped in the case of a cyclically varying bulk dipole moment (Sec. 2.3.6).

**Symmetries**

The quadrupole moment $q_{xy}$ in 2D is even under the group $T(2)$, which contains the operations $\{1, C_4M_x, C_4M_y, C_4^2\}$ (see Sec. 2.2.5), where $M_x$ and $M_y$ are reflections, and $C_4$ is the rotation by $\pi/2$ around the $z$ axis. This implies that none of the symmetries $\{C_4M_x, C_4M_y, C_4^2\}$ quantize the quadrupole moment $q_{xy}$ in crystalline insulators. On the other hand, the reflection operations $M_x, M_y$, and $C_4$, transform $q_{xy}$ to $-q_{xy}$. Hence, crystalline insulators with vanishing bulk dipole moment having any of $\{M_x, M_y, C_4\}$ will have a well-defined,
quantized quadrupole moment, though most insulators may simply just have a vanishing moment.

The quadrupole model with Bloch Hamiltonian (2.156) has the reflection symmetries of (2.89) with operators

\[
\hat{M}_x = i\tau_1 \otimes \tau_3, \quad \hat{M}_y = i\tau_1 \otimes \tau_1,
\]

as well as \(C_2\) symmetry

\[
\hat{r}_2 \hat{h}^q(k) \hat{r}_2^{-1} = \hat{h}^q(-k)
\]

with the \(C_2\) rotation operator

\[
\hat{r}_2 = \hat{M}_x \hat{M}_y = -i\tau_0 \otimes \tau_2.
\]

Notice that \(C_2\) symmetry for this model resembles the inversion symmetry (2.95). The reflection and \(C_2\) operators obey \(\hat{M}_x^2, \hat{M}_y^2 = -1\) and \(\hat{r}_2^2 = -1\). The point group of \(\hat{h}^q(k)\) in (2.156) is thus the quaternion group

\[
Q = \left\{ \bar{e}, \hat{M}_x, \hat{M}_y, \hat{r}_2 \mid \bar{e}^2 = 1, \hat{M}_x^2 = \hat{M}_y^2 = \hat{r}_2^2 = \hat{M}_x \hat{M}_y \hat{r}_2 = \bar{e} \right\}
\]

with \(\bar{e} = -1\). The quaternion group is of order 8, with elements \(\{ \pm 1, \pm \hat{M}_x, \pm \hat{M}_y, \pm \hat{r}_2 \}\). The three operators in (2.158) and (2.160) each have eigenvalues \(\{-i, -i, +i, +i\}\). Due to the \(\pi\)-flux threading each plaquette, the reflection operators do not commute, instead, they obey

\[
[\hat{M}_x, \hat{M}_y] = -2i\tau_0 \otimes \tau_2, \quad \{\hat{M}_x, \hat{M}_y\} = 0.
\]

The energy band degeneracy is protected at the high symmetry points of the BZ by the non-commutation of the reflection operators \(\hat{M}_x, \hat{M}_y\). Thus, it is not possible to lift the twofold degeneracy of the energy bands at those points while preserving both reflection symmetries. Indeed, at each of the high-symmetry points of the BZ, the subspace of occupied bands lies in the two-dimensional representation of the quaternion group.

Since \(C_2\) transforms the Bloch Hamiltonian \(\hat{h}^q(k)\) the same way as \(\mathcal{I}\) does, \(C_2\) symmetry quantizes the bulk dipole moment in \(\hat{h}^q(k)\) to \(p = 0\), as required for an insulator with well-defined quadrupole moment. \(M_x\) or \(M_y\) then quantize the quadrupole moment of \(\hat{h}^q(k)\) to either \(q_{xy} = 0\) or \(\frac{1}{2}\). The three symmetries in \(\hat{h}^q(k), M_x, M_y,\) and \(C_2\) are simultaneously present due to the fact that the existence of two of them implies the existence of the third one.
Alternatively, $C_4$ also quantizes $q_{xy}$. If we set $\gamma_x = \gamma_y$ and $\lambda_x = \lambda_y$, $h^q(k)$ has also $C_4$ symmetry,

$$\hat{r}_4 h^q(k) \hat{r}_4^{-1} = h^q(R_4 k), \quad \hat{r}_4 = \begin{pmatrix} 0 & \tau_0 \\ -i\tau_2 & 0 \end{pmatrix},$$

(2.163)

where $R_4$ is the rotation by $\pi/2$ of the crystal momentum, i.e., $R_4(k_x, k_y) = (k_y, -k_x)$. The $C_4$ rotation operator obeys $\hat{r}_4^2 = \hat{r}_2$ and $\hat{r}_4^4 = -1$ (the minus sign is due to the flux per unit cell) and has eigenvalues $\{e^{\pm i\pi/4}, e^{\pm 3i\pi/4}\}$.

Finally, $h^q(k)$, as written in Eq. (2.156), lies in class BDI, i.e., it has time-reversal, chiral and charge conjugation symmetries

$$\hat{T} h^q(k) \hat{T}^{-1} = h^q(-k), \quad \hat{T} = K$$

$$\Pi h^q(k) \Pi^{-1} = -h^q(k), \quad \Pi = \Gamma^0$$

$$Ch^q(k) C^{-1} = -h^q(-k), \quad C = \Gamma^0 K.$$  

(2.164)

However, these symmetries are not necessary for quantization of the quadrupole moment. In fact, we can break all of these symmetries and still preserve the quantization of the quadrupole observables as long as the reflection symmetries are preserved.

**Boundary signatures of the quadrupole phase**

Equation (2.128) gives the physical signatures of the quadrupole phase. With open boundaries, edge-localized polarizations exist, which can generate observable charge or currents as indicated by

$$Q^\text{edge}_a = -\partial_j p^\text{edge}_j^a, \quad J^\text{edge}_j^a = \partial_t p^\text{edge}_j^a.$$  

(2.165)

When two perpendicular boundaries are open, the edge polarizations along the boundaries generate a quadrupole pattern (see Fig. 2.3), and the corner hosts charges having the same magnitude as the edge polarizations. To illustrate these symmetry-protected signatures it will be convenient to use the Hamiltonian (2.156) in the limit $\gamma_x = \gamma_y = 0$, as shown in Fig. 2.21(a). In this limit, it is straightforward to identify the localized 1D boundary TIs associated with the edge polarization by eye, as well as the degenerate, mid-gap modes responsible for the corner charges.

Before we proceed, we point out a common subtlety in the calculation of electric moments. In the symmetry-protected topological phases with quantized quadrupole moment, the observables are not unam-
biguously defined, e.g., a value of $q_{xy} = \frac{1}{2}$ is equivalent to a value of $-\frac{1}{2}$, and similarly for $p_{\text{edge}}$ and $Q_{\text{corner}}$. This occurs when $h^q(k)$ has the quantizing symmetries that transform $q_{xy}$ to $-q_{xy}$. In order to unambiguously calculate the observables of the quadrupole insulator in a many-body ground state, we infinitesimally break all the symmetries that quantize the quadrupole so it will evaluate to a number close to, but not equal to, either $\frac{1}{2}$ or $-\frac{1}{2}$, as was done to fix the sign of the signatures in the SSH model (Sec. 2.3) and insulator $h^1(k)$ (Sec. 2.5). For that purpose, we consider the Hamiltonian

$$h^q_\delta(k) = h^q(k) + \delta \Gamma_0, \quad (2.166)$$

where $h^q(k)$ is the pristine, reflection-symmetric Hamiltonian in Eq. (2.156) with quantized boundary signatures, and $\Gamma_0 = \tau_3 \otimes \tau_0$ represents an on-site potential with the pattern shown in Fig. 2.21(b). This potential obeys $[\Gamma^0, M_x] \neq 0$, $[\Gamma^0, \tilde{M}_y] \neq 0$, and $[\Gamma^0, \tilde{r}_2] = 0$. It breaks the quantizing reflection symmetries of the quadrupole moment, but, crucially, retains $C_2$ symmetry, which maintains a vanishing, quantized value of the bulk dipole moment. In this section, we will keep $\delta \ll \gamma_x, \gamma_y, \lambda_x, \lambda_y$.

*Edge polarization:* A direct consequence of the nontrivial bulk topology of the quadrupole phase is the existence of edge polarization parallel to the edge. Consider first the quadrupole insulator in the limit $\gamma_x = \gamma_y = 0$ of Eq. (2.166), with $\delta \ll \lambda_x = \lambda_y \equiv \lambda$, and having open boundaries along $x$ but closed along $y$, as shown in Fig. 2.22(a). In the bulk, the electrons are connected via hopping on the square plaquettes, and form hybridized orbitals localized on the squares [shaded squares in Fig. 2.22(a)]. The overall electronic displacement in these plaquettes is zero. At the edges, however, electrons are only connected vertically as in the 1D symmetry-protected dipole phase of the SSH model [compare red and blue edges of Fig. 2.22(a) with Fig. 2.7(b)]. The small value of $\delta$ breaks the reflection symmetries and infinitesimally displaces the electrons away from $\frac{1}{2}$ to ‘choose a sign’ for the edge polarizations, as shown in the first plot of Fig. 2.22(b), where we plot the polarization along $y$ resolved in space along $x$, $p_y(R_x)$ [this is calculated using the prescription
in Sec. 2.5 that results in Eq. (2.126)]. If we turn on $\gamma_x$ and $\gamma_y$, the edge polarization remains quantized to $\frac{1}{2}$ (although it exponentially penetrates into the bulk), as long as $|\gamma_x/\lambda_x| < 1$ and $|\gamma_y/\lambda_y| < 1$, as shown in the second plot of Fig. 2.22(b). If, on the other hand, $|\gamma_x/\lambda_x| > 1$ or $|\gamma_y/\lambda_y| > 1$, the edge polarization drops to zero, as seen in the third plot of Fig. 2.22(b).

*Corner charge:* In the quadrupole insulator with full open boundaries, the edge-localized dipole moments will accumulate corner charge. If edge dipole moments per unit length of $q$ exist, we would expect a corner charge $\pm 2q$. However, the corner charge in the quadrupole insulator $h^q(\mathbf{k})$ has equal magnitude to the edge-polarization, i.e., $q$, following (2.128). Hence, since the contributions from edge dipole moments alone over-count the corner charge, there has to be an additional direct contribution from the bulk to the corner charge.

The different contributions to the corner charge can be clearly illustrated in the limit $\gamma_x = \gamma_y = 0$, shown in Fig. 2.23(a). The large blue circles represent an ionic charge of $+2e$, which is constant across unit cells. Each unit cell has four electronic degrees of freedom, and thus, at half-filling, each unit cell contributes two electrons. The sites connected by lines represent localized hybrid orbitals of the occupied electrons in the many-body ground state. In the bulk there are two localized square orbitals on each inter-cell plaquette, and the electrons in these orbitals have equal weight on each site of the plaquette. On the edges there are localized inter-cell dimer orbitals, one per dimer, where the electrons have equal weight on each site of the dimer. In this limit where $\gamma_x = \gamma_y = 0$, each of the green sites in the bulk has an electronic charge of $-\frac{e}{2}$ coming from the two square-localized orbitals, each contributing $1/4$ of an electron. Similarly, each of the green sites on the edge SSH chains has an electronic charge of $-\frac{e}{2}$. Finally, there are two red and two white circles at the corners. Each of these degrees of freedom is decoupled from the rest in this limit and therefore
Figure 2.23: Corner charge in the quadrupole insulator. (a) Schematic of charge in the limit $\gamma_x = \gamma_y = 0$ when an infinitesimal perturbation as in Fig. 2.21(b) is included. The lines connecting sites represent localized hybrid electron orbitals in the many-body ground state at half-filling. This is an exact representation of the ground state in the zero-correlation length limit. Each blue, green, and red circle represents charges of $+2e$ (ionic), $-e/2$, and $-e$, respectively. White circles do not have charge. (b) Simulation of the charge density for $\lambda_x = \lambda_y = 1$, $\gamma_x = \gamma_y = 10^{-3}$, and $\delta = 10^{-3}$. Sites in the square plaquette orbitals marked with a $*$ closest to them represent half-charge contributions to the corner charge from the bulk orbitals.

have exactly zero energy. These are the corner modes associated with the fractional corner charge in the topological quadrupole phase. Out of the four mid-gap corner modes, two should be filled at half-filling. A small value of $\delta \ll \lambda_x, \lambda_y$ in (2.166) breaks this degeneracy in a manner where $C_2$ symmetry is preserved, and specifies which modes are to be filled. When $\delta > 0$, each of the red circles is occupied since they are at lower energy than the white circles. Thus each red circle contributes $-e$ to the charge at its corner unit cell. The white circles, on the other hand, remain unoccupied and do not contribute to the electronic corner charge. Notice that in the bulk and the edges, the positive atomic charge cancels the electronic charge. In the corner unit cells, however, there is a total charge of $\pm \frac{e}{2}$. Just as in the case of the edge polarization, the corner charge persists as long as $|\gamma_x/\lambda_x| < 1$ and $|\gamma_y/\lambda_y| < 1$, and drops to zero otherwise. An example of the distribution of electronic charge density for $\gamma_x \neq 0$ and $\gamma_y \neq 0$ is shown in Fig. 2.23(b).

The Hamiltonian (2.156) in the limit $\gamma_{x,y} = 0$, shown in Fig. 2.23(a), illustrates two important characteristics of the quadrupole: (i) the fractionalization of the corner charge does not come from the edge polarizations alone, i.e., the contributions due to the nontrivial polarizations give an overall integer contribution to the corner charge. The fractionalization of the corner charge comes from the bulk charge density, and in this simple limit it comes from the corners of the plaquette orbitals that are closest to the corners [circles marked with a $*$ in Fig. 2.23(a)]. (ii) Despite the existence of two topological edge dipoles meeting at each corner in the nontrivial phase, there is only one zero-energy state per corner. This is contrary to the conventional notion that a domain between two SSH chains, both of which are in the topological phase, should not trap a stable mid-gap mode. The apparent paradox is resolved because the protected topological corner state is a simultaneous eigenstate of both edge Hamiltonians along the $x$ and $y$ edges. This is evident in the pictorial representation of Fig. 2.23(a), but can be confirmed in a more general setting by an explicit
calculation of the corner-localized eigenstate. To demonstrate this, let us begin with our lattice Hamiltonian (2.156) with $\lambda = 1$:

$$h^q(k) = \sin k_x \Gamma_3 + (\gamma_x + \cos k_x) \Gamma_4 + \sin k_y \Gamma_1 + (\gamma_y + \cos k_y) \Gamma_2.$$  

(2.167)

To simplify the present discussion, we will solve a continuum version of the Hamiltonian by assuming that $\gamma_x = -1 + m_x$ and $\gamma_y = -1 + m_y$ for $m_{x,y}$ small and positive (negative) for the topological (trivial) phase. We can take a continuum limit, or equivalently a $k \cdot p$ expansion about $(k_x, k_y) = 0$, to find the Hamiltonian

$$H = k_x \Gamma_3 + m_x \Gamma_4 + k_y \Gamma_1 + m_y \Gamma_2.$$  

(2.168)

We now use this Hamiltonian to solve for the states localized on the $x$ edge, and then project the Hamiltonian into these states to form the $x$-edge Hamiltonian, from which we can then calculate the corner states. We will treat the $x$ edge as a domain wall where $m_x$ steps from positive (inside the topological phase) to negative (outside the topological phase), and the $y$ edge as a domain wall where $m_y$ steps from positive to negative, as shown in Fig. 2.24. We use the ansatz $\Psi(x, k_y) = f(x) \Phi_x(k_y)$ for the wave function localized at the $x$ edge in the absence of $y$ edges. In this ansatz, $f(x)$ is a scalar function of $x$ and $\Phi_x(k_y)$ is a spinor which depends on $k_y$. By inserting this ansatz into the Schrödinger equation with Hamiltonian (2.168) and dividing by $f(x)$ we have

$$\left(-i \frac{\partial_x f(x)}{f(x)} \Gamma_3 + m_x(x) \Gamma_4\right) \Phi_x(k_y) + (k_y \Gamma_1 + m_y \Gamma_2) \Phi_x(k_y) = c \Phi_x(k_y),$$  

(2.169)
where we have replaced $k_x \to -i\partial_x$, and $\epsilon$ is the energy. Since the first term in parentheses has all the dependence on $x$, Eq. (2.169) only has a solution if the first term is a constant. In particular, we choose that constant to be zero (a different value only redefines the zero-point energy of the Hamiltonian),

$$( -i\partial_x \Gamma_3 + m_x(x)\Gamma_4 ) f(x) \Phi_x(k_y) = 0.$$  \hfill{(2.170)}

This has the solution $f(x) = C \exp(\int_0^x m_x(x')dx')$, with normalization constant $C$. The matrix equation that results from solving (2.170) can be simplified to $(I - \tau^z \otimes \sigma^z)\Phi_x = 0$, from which follows that $\Phi_x$ is a positive eigenstate of $\tau^z \otimes \sigma^z$, i.e., $\Phi_{x1} = (1, 0, 0, 0)$ or $\Phi_{x2} = (0, 0, 0, 1)$. We now project the remaining part of the Hamiltonian into the subspace spanned by these two states to find the low-energy Hamiltonian of the $x$-edge

$$H_{edge,x} = -k_y \mu^y + m_y \mu^x,$$  \hfill{(2.171)}

where $\mu^a$ are Pauli matrices in the basis $(\Phi_{x1}, \Phi_{x2})$.

Performing an analogous calculation for the $y$ edge, we find the matrix equation $(I - I \otimes \sigma^z)\Phi_y = 0$, which has solutions that are positive eigenstates of $I \otimes \sigma^z$, i.e., $\Phi_{y1} = (1, 0, 0, 0)$ or $\Phi_{y2} = (0, 0, 1, 0)$. We then project the remaining bulk terms into this basis to find the $y$-edge Hamiltonian

$$H_{edge,y} = -k_x \gamma^y + m_x \gamma^x,$$  \hfill{(2.172)}

where $\gamma^a$ are Pauli matrices in the basis $(\Phi_{y1}, \Phi_{y2})$.

Both of these edge Hamiltonians take the form of massive $(1+1)$D Dirac models, i.e., the natural minimal continuum model for a $(1+1)$D topological insulator (an alternative analysis arriving at this conclusion is found in Ref. [87]). Now, the key feature we mentioned earlier, i.e., the simultaneous zero-energy state can be found by considering a corner, i.e., either the $x$ edge with a $y$-domain wall or the $y$ edge with a $x$-domain wall.

Let us first look for the zero-energy states localized at a $y$-domain wall on the upper portion of a vertical 1D chain with Hamiltonian (2.171). The ansatz in this case is of the form $\Phi_x(y) = \exp(\int_0^y m_y(y')dy')\phi_{x,y}$, which, from the Schrödinger equation for Hamiltonian (2.171), and choosing zero energy, leads to a matrix equation that simplifies to

$$(I - \mu^z)\phi_{x,y} = 0.$$  \hfill{(2.173)}
Using similar calculations to those above we find the following matrix equation for the $x$-domain wall on the right side of a horizontal 1D insulator with Hamiltonian (2.172):

$$(\mathbb{I} - \gamma^z)\phi_{y,x} = 0.$$  \hspace{1cm} (2.174)

Hence, the corner state we find for an $x$ edge with a $y$ domain wall is the positive eigenstate of $\mu^z$ while that for the $y$-edge with an $x$ domain wall is the positive eigenstate of $\gamma^z$. In both cases the solutions are identical, i.e., they are the first basis elements $\Phi_{x1} = \Phi_{y1} = (1, 0, 0, 0)$. Therefore, the corner zero-energy state is a simultaneous state of both domain wall Hamiltonians, given by

$$\Psi_{\text{corner}}(x, y) = e^{\int_0^x m_z(x')dx'} e^{\int_0^y m_y(y')dy'} (1, 0, 0, 0).$$  \hspace{1cm} (2.175)

Thus, although both edges are 1D topological insulators, they only produce a single zero mode. Indeed, the corner states are not traditional 1D domain wall states, and represent a new mechanism to generate such modes on the boundary of a 2D system.

In order to understand how the boundary polarization arises in the topological quadrupole phase, it is useful to study the topology of the Wannier bands, and how this topological structure manifests at boundaries. We focus on this in the following three sections.

**Topological classes of the Wannier bands**

Under $M_x$, $M_y$ and $C_2$, the Wannier-sector polarizations obey the relations in Eq. (2.146). In the quadrupole insulator $h^q(k)$, these relations imply that: (i) all the Wannier-sector polarizations, $p_x^\nu$ and $p_y^\nu$, are quantized [see Eq. (2.147)], and (ii) out of these four polarizations two are redundant due to $C_2$ symmetry. Specifically, we can re-write the third expression in (2.146) as

$$p_x^+ + p_x^- \equiv 0 \mod 1, \quad p_y^+ + p_y^- \equiv 0 \mod 1,$$

which is the statement that the total dipole moment vanishes, as is needed for a well defined quadrupole moment (see Sec. 2.2.2),

$$\mathbf{p} = (p_x, p_y) = 0.$$  \hspace{1cm} (2.177)
Figure 2.25: Diagram of topological classes for the Wannier bands of the insulator $h^q(k)$ with Bloch Hamiltonian Eq. (2.156). The indices $p^\nu$ are defined in Eq. (2.178). The trivial class has $p^\nu = (0, 0)$.

where

$$p_x = p_x^\nu + p_x^{\nu -}$$

and

$$p_y = p_y^\nu + p_y^{\nu -}.$$  

Due to the relations (2.176), only two independent Wannier-sector polarizations are necessary to specify the topological class of the Wannier bands, and we can define the index

$$p^\nu \equiv (p_x^{\nu -}, p_y^{\nu -}).$$  

(2.178)

Under $M_x$, $M_y$ and $C_2$, the classification of the Wannier band topology in $h^q(k)$ is $\mathbb{Z}_2 \times \mathbb{Z}_2$. A diagram of these classes is shown in Fig. 2.25 as a function of the ratios $\gamma_x/|\lambda_x|$ and $\gamma_y/|\lambda_y|$. The central square of the diagram in the ranges $\gamma_x/|\lambda_x| \in [-1, 1]$ and $\gamma_y/|\lambda_y| \in [-1, 1]$ is the region in parameter space having $p^\nu = (\frac{1}{2}, \frac{1}{2})$. Additionally, there are two regions in parameter space with $p^\nu = (0, \frac{1}{2})$, and two more with $p^\nu = (\frac{1}{2}, 0)$, as well as four regions in the trivial topological class $p^\nu = (0, 0)$.

In the presence of reflection symmetries, $p^\nu$ can be determined by the reflection representation of the Wannier bands at the high-symmetry lines

$$\hat{M}_y \left| w_{x, (k_x, k_{xy})}^\pm \right> = \alpha_{M_y}^\pm (k_x, k_{xy}) \left| w_{x, (k_x, k_{xy})}^\pm \right>$$

$$\hat{M}_x \left| w_{y, (k_x, k_y)}^\pm \right> = \alpha_{M_x}^\pm (k_{sx}, k_y) \left| w_{y, (k_x, k_y)}^\pm \right>,$$  

(2.179)

for $k_{sx,y} = 0, \pi$ (see Sec. 2.6.2). In the $p^\nu = (\frac{1}{2}, \frac{1}{2})$ class, the values of $\alpha_{M_x}^\pm (k_{sx}, k_y)$ and $\alpha_{M_y}^\pm (k_x, k_{sy})$ are shown in Fig. 2.26. For each of the topological classes of the Wannier bands shown in Fig. 2.25, the corresponding $\alpha$ values are shown in Table 2.5. Using these values we can evaluate the Wannier-sector polarizations according to Eq. (2.149). In $h^q(k)$, these lead to the Wannier-sector polarization (for the lower Wannier bands) shown in the phase diagram in Fig. 2.25.
$p^\nu = (\frac{1}{2}, \frac{1}{2}) \quad p^\nu = (\frac{1}{2}, 0) \quad p^\nu = (0, \frac{1}{2})$

<table>
<thead>
<tr>
<th>$\alpha^+_{M_x}(0, k_y)$</th>
<th>$\alpha^+_{M_y}(k_x, k_y)$</th>
<th>$\alpha^-_{M_x}(0, k_y)$</th>
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Table 2.5: Reflection eigenvalues of lower Wannier bands in the different topological classes of the Wannier bands of the Hamiltonian in Eq. (2.156). The upper (lower) values in the $p^\nu = (\frac{1}{2}, 0)$ phase correspond to the upper (lower) blocks in the phase diagram in Fig. 2.25, while the upper (lower) values in the $p^\nu = (0, \frac{1}{2})$ phase correspond to the blocks to the left (right) in the phase diagram in Fig. 2.25.

Figure 2.26: Reflection eigenvalues $\alpha^+_{M_y}(k_x, k_{xy})$ (red signs) and $\alpha^+_{M_x}(k_x, k_y)$ (blue signs) of the Wannier bands of the occupied energy bands in the topological quadrupole phase. Here $k_{*x,y} = 0, \pi$. For the unoccupied bands, all signs are inverted.

Transitions between the topological classes of Wannier bands

At the transitions between topological classes indicated in Fig. 2.25, the Wannier gap closes. This is analogous to the closing of the energy gap in phase transitions between distinct symmetry-protected topological phases. Figure 2.27 shows the momentum and Wannier value locations at which the Wannier gap closes at all the topological class transitions in Fig. 2.25. With reflection symmetries $M_x$ and $M_y$, the Wannier gap can close at two Wannier values, $\nu = 0$ or $\frac{1}{2}$. Consider, for example, the path in parameter space shown by the red line in Fig. 2.27 that starts in the $p^\nu = (\frac{1}{2}, \frac{1}{2})$ class and ends in the trivial class $p^\nu = (0, 0)$ via the intermediate class $p^\nu = (\frac{1}{2}, 0)$. In Fig. 2.28 we plot the two Wannier bands for each of the five Hamiltonians corresponding to the red dots in Fig. 2.27. In the $p^\nu = (\frac{1}{2}, \frac{1}{2})$ class, both Wannier bands are gapped and nontrivial. At the first transition point, the Wannier bands $\nu_x(k_y)$ become gapless at $k_y = \pi$ as they become twofold degenerate at $\nu_x(k_y = \pi) = \frac{1}{2}$. The bands $\nu_y(k_x)$, on the other hand, remain gapped at all $k_x \in (-\pi, \pi]$. On the other
Figure 2.27: Diagram of Wannier band transitions in model (2.156). At transitions there is Wannier gap closing at either $\nu_x(k_y = 0, \pi) = 0$ or $\nu_y(k_x = 0, \pi) = 0$ (dashed lines) or at either $\nu_x(k_y = 0, \pi) = \frac{1}{2}$ or $\nu_y(k_x = 0, \pi) = \frac{1}{2}$ (solid thick lines).

side of this transition, in the $p^{\nu} = (\frac{1}{2}, 0)$ class, the Wannier bands $\nu_x(k_y)$ become gapped again, but this time they have trivial topology (i.e., $p^{\nu}_{\nu} = 0$).

As the $p^{\nu} = (\frac{1}{2}, 0)$ class approaches the transition into the trivial class $p^{\nu} = (0, 0)$, another Wannier gap closing event occurs. This time, however, it is the $\nu_y(k_x)$ bands that close the gap at the $k_x = \pi$ point. They acquire the twofold-degenerate value of $\nu_y(k_x = \pi) = 0$. On the other side of the transition, in the trivial class, both Wannier bands are gapped and have trivial topology. At transitions from the $p^{\nu} = (\frac{1}{2}, \frac{1}{2})$ class to the trivial class $p^{\nu} = (0, 0)$ other than the one indicated by the red line in Fig. 2.28, transitions can occur by closing the Wannier gaps of $\nu_y$ ($\nu_x$) at $k_x = 0$ or $\pi$ ($k_y = 0$ or $\pi$), as indicated in Fig. 2.27. In all cases, however, the Wannier gap always closes at the value $\nu = \frac{1}{2}$ as it leaves the $p^{\nu} = (\frac{1}{2}, \frac{1}{2})$ class to either the $p^{\nu} = (0, \frac{1}{2})$ or $p^{\nu} = (\frac{1}{2}, 0)$ classes, and then at the value $\nu = 0$ from these classes to the trivial $p^{\nu} = (0, 0)$ class. This is not accidental.

**Bulk-boundary correspondence for Wannier bands and edge polarization**

We saw that transitions between different topological classes of Wannier bands close the Wannier gap. Therefore, at a physical boundary between insulators having different Wannier classes, the Wannier gap is also expected to close. We denote this property as a bulk-boundary correspondence for Wannier bands. Consider, for example, the quadrupole insulator (2.155) with closed boundaries along $x$ and open along $y$.  

75
By redefining the unit cell of this 2D crystal to get an effective 1D crystal with a unit cell of \( N \text{_{orb}} \times N_y \) sites, we can obtain a Bloch Hamiltonian \( h^q(k_x) \), with only one crystal momentum \( k_x \). We write \( h^q(k_x) \) to differentiate it from the Bloch Hamiltonian \( h^q(k) = h^q(k_x, k_y) \), which has full periodic boundaries. While \( h^q(k) \) has Wilson loops \( \mathcal{W}_{x,k} \) with Wannier bands \( \nu^\pm_x(k_y) \), \( h^q(k_x) \) has Wilson loops \( \mathcal{W}_{x,k_x} \) with Wannier values \( \nu^j_x \), for \( j = 1 \ldots 2N_y \) (at half-filling), as defined in Sec. 2.5.

The bulk-boundary correspondence for Wannier bands then implies that, if the Wannier bands \( \nu^\pm_x(k_y) \) of \( h^q(k) \) have nontrivial topology, i.e., if \( p_{y}^{\nu^\pm_x} = \frac{1}{2} \), there will be \( y \)-edge-localized eigenstates of the Wilson loop \( \mathcal{W}_{x,k_x} \) of \( h^q(k_x) \) with eigenvalue \( \nu_x = 0 \) or \( \frac{1}{2} \) (as protected by \( M_x \)). We denote these as Wannier edge states. Hence, the Wannier values of the insulator with open boundaries along \( y \) are gapless, and the gapless states are localized at the edges. If, on the other hand, \( p_{y}^{\nu^\pm_x} = 0 \), then there are no edge-localized eigenstates of \( \mathcal{W}_{x,k_x} \); i.e., no Wannier edge states. For the former case in which \( p_{y}^{\nu^\pm_x} = \frac{1}{2} \), the Wannier edge states, localized at \( R_y = 0 \) and \( R_y = N_y \), are extended along \( x \). Their Wannier value, which is either \( \nu_x = 0 \) or \( \frac{1}{2} \), indicates their dipole moment along \( x \). These modes are thus responsible for the edge-localized polarization parallel to the edge. Whether the topological Wannier edge modes have \( \nu_x = 0 \) or \( \frac{1}{2} \) (the only two allowed values under \( M_x \)) is determined by the value of \( p_{x}^{\nu^\pm_x} \).

The connection between the bulk property \( p_{y}^{\nu^\pm_x} = \frac{1}{2} \) and the existence of Wannier edge states can be seen as follows. The bulk Wannier bands \( \nu^\pm_x(k_y) \), being gapped, allow us two define two maximally-localized Wannier centers along \( x \): one arising from the \( \nu^+_x \) Wannier sector, which is localized to the right (horizontally) of the center of the unit cell, and another arising from the \( \nu^-_x \) Wannier sector, which is localized to the left.
Figure 2.29: Representative tight-binding Hamiltonians, Wannier values \( \{ \nu_j^x \} \), for \( j = 1 \ldots 2N_y \), and polarization \( p_y(R_y) \) for all topological classes \( \mathbf{p}^\nu \) of \( \hat{h}^\theta(k) \). The tight-binding Hamiltonians have closed boundaries along \( x \) and open along \( y \), and are drawn with \( \gamma_x, \gamma_y, \lambda_x, \lambda_y = 0 \) whenever possible to ease the visualization of the edge states and edge polarizations. The Wannier values \( \{ \nu_j^x \} \) and polarizations \( p_x(R_y) \) are calculated in the same topological class as the Hamiltonians on their left, but with parameters \( \lambda_x = \lambda_y = 1 \) in all four cases and \( (\gamma_x, \gamma_y) = (1.25, 0.25) \) in (a), \( (\gamma_x, \gamma_y) = (0.25, 0.25) \) in (b), \( (\gamma_x, \gamma_y) = (1.25, 1.25) \) in (c), and \( (\gamma_x, \gamma_y) = (0.25, 1.25) \) in (d). (a) and (b) have pairs of Wannier edge states (red thick circles) with degenerate values \( \nu_x = 0 \) and \( \nu_x = \frac{1}{2} \), respectively. (c) and (d) do not have Wannier edge states. Only (b) has a nontrivial edge polarization and quantized quadrupole moment. A value of \( \delta = 10^{-3} \) was set in the calculation of \( p_x(R_y) \) for all cases to choose the sign of the quadrupole.

(horizontally) of the center of the unit cell. \( p_y^\nu = \frac{1}{2} \) tells us that each of these Wannier centers is displaced by half of a unit cell along \( y \), hence giving rise to Wannier edge states when the system’s boundaries are opened. When \( p_y^\nu \) is exactly quantized, which Wannier center of the \( \nu_x^\pm \) Wannier bands is displaced up or down is ambiguous in the bulk of the insulator. However, when the boundaries are open, \( C_2 \) symmetry guarantees that there will be one Wannier edge state on each of the lower and upper surfaces (as opposed to, say, two edge modes on the upper surface and none on the lower).

The properties described above can be visualized in Fig. 2.29, which shows the simplest tight-binding Hamiltonians (by setting \( \gamma_x, \gamma_y, \lambda_x, \lambda_y = 0 \) whenever possible) in all of the four Wannier classes of \( \hat{h}^\theta(k) \). Next to each of the tight-binding lattices we show the Wannier values \( \{ \nu_j^x \} \), for \( j = 1 \ldots 2N_y \) (i.e., the eigenvalues of \( W_{x,k_x} \)), for \( \hat{h}^\theta(k_x) \) in the same Wannier-band topological class, as well as their resulting polarizations \( p_x(R_y) \).

In the cases in which \( p_y^\nu = \frac{1}{2} \) [Figs. 2.29(a) and 2.29(b)], \( 2N_y - 2 \) states are spread over the bulk, while two (the topological Wannier edge states) are localized on the edges; one at \( R_y = 0 \) and the other one at \( R_y = N_y \). These two Wannier edge states have dipole moments along \( x \) equal to the value of \( p_x^\nu \). For \( p_x^\nu = 0 \) [Fig. 2.29(a)] the edge states have zero dipole moment; note by inspection of the tight-binding
lattice that the edge states are each an SSH chain in the trivial phase. For $p_x^{ν_±}=\frac{1}{2}$ [Fig. 2.29(b)], the edge states have nontrivial, half-integer dipole moment; note by inspection of the tight-binding lattice that these edge states are each an SSH chain in the nontrivial phase.

When $p_y^{ν_±}=0$, on the other hand, there are no Wannier edge states in the $W_{x,k_x}$ spectrum of $h^q(k_x)$. This is independent of the value of $p_x^{ν_±}$ [Figs. 2.29(c) and 2.29(d)]. Thus, whether the Wanner bands $ν_y^{±}(k_x)$ are trivial or topological [Fig. 2.29(c) and 2.29(d), respectively], the absence of Wannier edge states automatically leads to a vanishing dipole moment along $x$ at both $y$-edges.

From the analysis above it follows that, of all the four classes in $h^q(k)$, only the class $p^{ν}=\left(\frac{1}{2}, \frac{1}{2}\right)$ exhibits nontrivial edge polarization. Correspondingly, only this class has corner-localized charges of $\frac{1}{2}$ when the boundaries along both $x$ and $y$ are open. Hence, only the $p^{ν}=\left(\frac{1}{2}, \frac{1}{2}\right)$ class has nontrivial quantized quadrupole moment $q_{xy}=\frac{1}{2}$, while all the other three classes have trivial quantized quadrupole moment $q_{xy}=0$.

**Topological phases in the quadrupole insulator**

Now that we have identified which Wannier topological classes (in the presence of $M_x$ and $M_y$) have nontrivial quadrupole moments, we look into the symmetry-protected topological quadrupole phases. The quadrupole insulator has a quantized phase protected not only by $M_x$ and $M_y$, but also by $C_4$ symmetry. That is, we could choose either the combination of $M_x$ and $M_y$ or $C_4$ to protect the quadrupole moment. We analyze these two types of protection separately.

**Reflection symmetric phases** A diagram of the topological quadrupole phases of the insulator $h^q(k)$ is shown in Fig. 2.30 as a function of the ratios $γ_x/|λ_x|$ and $γ_y/|λ_y|$. The central square of the diagram in the ranges $γ_x/|λ_x| \in (-1, 1)$ and $γ_y/|λ_y| \in (-1, 1)$ has a quantized quadrupole moment $q_{xy}=\frac{1}{2}$, as it has the boundary signatures of Eq. (2.128). Outside of this region, there is a trivial quantized quadrupole $q_{xy}=0$.

Following the paradigm for the topological characterization of crystalline symmetry-protected topological phases [31, 33, 18, 19, 34, 36, 37, 49], we look at the symmetry group representations that the subspace of occupied bands takes at the high-symmetry points of the BZ. The point group of the quadrupole insulator $h^q(k)$ is the quaternion group (2.161). This group has 4 one-dimensional representations and one two-dimensional representation. The points of the BZ invariant under this group are $k_*=Γ, X, Y, M$. At all of these points, there is a twofold degeneracy in the spectrum protected by the non-commutation of the $M_x$ and $M_y$ operators and the subspaces of occupied bands at these points lie in the only two-dimensional representation of the quaternion group. Symmetry-allowed perturbations can be added to lift most of the
Figure 2.30: Phase diagram of the quadrupole insulator $h^q(k)$ with Hamiltonian (2.156). Transitions close the bulk-energy gap when $C_4$ symmetry is preserved at the indicated points of the BZ. Transitions close the edge energy gap when $M_x$ and $M_y$ reflections are preserved at the indicated edges.

twofold degeneracy of the bulk energy bands of $h^q(k)$ [given in Eq. (2.157)], however the degeneracy will persist at all $k_*$ points of the BZ [Fig. 2.31(a)].

Since the quaternion group admits only one two-dimensional representation, one cannot construct the typical bulk crystalline topological invariants (the representations are the same at each $k_*$), and hence the topological structure is “hidden” from the point of view of the group representations of the energy bands. Instead, the topology in the presence of $M_x$ and $M_y$ is captured by the topological classes of the Wannier bands. The reflection and $C_2$ eigenvalues of the occupied energy bands at each $k_*$ all come in $(+i, -i)$ pairs. These values are necessary to have gapped Wannier bands, $\nu^\pm_x (k_y)$ and $\nu^\pm_y (k_x)$, as shown in Fig. 2.18 (pairs of reflection or $C_2$ eigenvalues other than $(+i, -i)$, inevitably lead to at least one pair of Wannier bands being gapless, see Sec. 2.6.3). The Wannier bands can belong to different topological classes, as discussed in Sec. 2.6.4, and are identified by a pair of Wannier-sector polarizations as in Eq. (2.178). Since the $q_{xy} = \frac{1}{2}$ phase coincides with the Wannier band topology having $p^y = (\frac{1}{2}, \frac{1}{2})$, we can construct the index for the reflection symmetry-protected quadrupole phase as

$$q_{xy}^{M_x; M_y} = \frac{\nu^y_y}{p_y} \frac{\nu^x_x}{p_x} + \frac{\nu^y_y}{p_y} \frac{\nu^x_x}{p_x}$$

(2.180)
which takes values

\[
q_{xy}^{M_xM_y} = \begin{cases} 
0, & \text{if trivial} \\
\frac{1}{2}, & \text{if nontrivial.}\end{cases}
\] (2.181)

The expression (2.180) resembles the classical expression for a quadrupole; it is the multiplication of two “coordinates” (one measures the displacement along \( x \) and the other one along \( y \)) added over the charges (two electrons in this case). Due to the constraint (2.176), the index simplifies to

\[
q_{xy}^{M_xM_y} = 2p_x^+p_y^- - p_x^-p_y^+.
\] (2.182)

Accordingly, both the edge polarizations and the corner charges of the insulator in this nontrivial SPT phase are quantized. The protection due to Wannier band topology, instead of bulk energy band topology, is a new mechanism of topological protection. This protection implies that, at symmetry-preserving boundaries between a topological phase and the vacuum, edges are not required to be gapless, i.e., it allows for the possibility of gapped edges. These edges, however, are topological themselves. The Wannier band protection mechanism leads to the existence of gapped, symmetry-preserving edges which are topological. This idea can be extended far beyond this example so that we can generate bulk topological phases with many types of gapped, surface SPTs. In some sense, these phases represent a simpler version of the gapped, symmetry-preserving surfaces of 3D strong topological phases which must instead be topologically ordered [88, 89, 90, 91, 92]

**C\(_4\)-symmetric phases** A schematic representation of a quadrupole with \( C_4 \) symmetry but not \( M_x \) or \( M_y \) symmetries is shown in Fig. 2.32. It is a variation of the insulator shown in Fig. 2.20, but here we set \( \gamma_x = \gamma_y = \gamma \) and \( \lambda_x = \lambda_y = \lambda \), and allow the fluxes threading each plaquette to be different than \( \pi \). The
Figure 2.32: Quadrupole model that preserves $C_4$ symmetry. Red (blue) plaquettes have flux $\varphi_0$ ($\varphi$). Plaquettes sharing red and blue couplings have a flux of $-(\varphi_0 + \varphi)/2$.

‘red’ plaquettes, delimited by the intra-cell $\gamma$ couplings have flux $\varphi_0$, while the ‘blue’ plaquettes, delimited by the inter-cell $\lambda$ hoppings have flux $\varphi$. To simplify the formulation, we take the fluxes into account by replacing

$$\gamma \rightarrow \gamma e^{i\varphi_0/4}, \quad \lambda \rightarrow \lambda e^{i\varphi/4}$$  \hspace{1cm} (2.183)

in the directions of the arrows in Fig 2.32, or their complex conjugate in the opposite direction. This implies that plaquettes sharing red couplings and blue hoppings have a flux of $-(\varphi + \varphi_0)/2$. When $\varphi = \varphi_0 = 0, \pi$ the insulators have reflection symmetries $M_x, M_y$. If $\varphi = \varphi_0 = 0$, we have $[\hat{M}_x, \hat{M}_y] = 0$, and the spectrum is gapless at half filling. If $\varphi = \varphi_0 = \pi$, on the other hand, we recover the insulator (2.156), which has $\{\hat{M}_x, \hat{M}_y\} = 0$, and realizes a quadrupole SPT phase. In Fig. 2.31(b), we show the energy spectrum for the values $\varphi_0 = 0, \varphi = \pi$. Since the anti-commuting reflection symmetries are lost, so is the protection of the degeneracies at the high-symmetry points of the BZ [cf. Fig. 2.31(a)]. The energy and Wannier bands remain gapped during the deformation $\varphi_0 = \pi \rightarrow \varphi_0 = 0$ that connects the quadrupole (2.156) with the Hamiltonian having the energy spectrum in Fig. 2.31(b). Thus, the nontrivial topology persists and the quadrupole is in either the trivial phase, $q_{xy} = 0$, or the topological phase, $q_{xy} = \frac{1}{2}$. Unlike the case in which symmetries $M_x$ and $M_y$ protect the quadrupole moment, under $C_4$ symmetry the quadrupole moment is protected by the topology of the bulk energy bands. Accordingly, a topological index can be built by comparing the rotation representations of the subspace of occupied energy bands at the $C_4$-symmetric points of the BZ, $k_s = \Gamma$ and $\mathbf{M}$ [36, 37], shown in Fig 2.33(a). Since $C_4$ symmetry only has one-dimensional representations, it does not protect degeneracies in the energy bands of $h^\gamma(\mathbf{k})$. In order to define the topological index, consider $h^\gamma(\mathbf{k}_s)$, with $\gamma_x = \gamma_y = \gamma$ and $\lambda_x = \lambda_y = \lambda$, which obeys

$$[\hat{r}_4, h^\gamma(\mathbf{k}_s)] = 0.$$  \hspace{1cm} (2.184)
Figure 2.33: Rotation representations for the occupied bands of the quadrupole model (2.156) in the presence of $C_4$ symmetry (2.163). (a) BZ and its $C_4$-invariant momenta $\mathbf{k}_* = \Gamma, M$ (b-d) Let $\lambda_x = \lambda_y = 1$, $\gamma_x = \gamma_y = \gamma$. $C_4$ rotation eigenvalues at $\mathbf{k}_*$ for (b) quadrupole phase, $|\gamma| < 1$, (c) trivial phase with $\gamma > 1$, and (d) trivial phase with $\gamma < -1$.

From this it follows that the eigenstates of $h^q(\mathbf{k}_*)$ are also eigenstates of the rotation operator. Thus, the occupied states at $\mathbf{k}_*$ obey

$$\hat{r}_4 |u^n_{\mathbf{k}_*}\rangle = r_4^n(\mathbf{k}_*) |u^n_{\mathbf{k}_*}\rangle,$$

where $n = 1, 2$ labels the occupied states, and $r_4^n(\mathbf{k}_*)$ is the rotation eigenvalue of the $n$th occupied state at the $C_4$-invariant momentum $\mathbf{k}_*$.

To build the index, we first recall that the eigenvalues of the $C_2$ operator, $\hat{r}_2 = \hat{r}_4^2$, for the occupied bands at the $\mathbf{k}_*$ are $\pm i$. Thus, the $C_4$ eigenvalues in the occupied energy bands come in pairs $r_4^+(\mathbf{k}_*), r_4^- (\mathbf{k}_*)$ obeying

$$(r_4^+(\mathbf{k}_*))^2 = +i, \quad (r_4^- (\mathbf{k}_*))^2 = -i. \quad (2.186)$$

With this restriction, there are only two topologically distinct configurations of eigenvalues as shown in Fig. 2.33. We can then take either the $r_4^+(\mathbf{k}_*)$ values or the $r_4^- (\mathbf{k}_*)$ values to construct the index

$$e^{i2\pi q_{xy}^*} \equiv r_4^+(\mathbf{M})r_4^+\ast(\Gamma) = r_4^- (\mathbf{M})r_4^-\ast(\Gamma), \quad (2.187)$$
Figure 2.34: Schematic of a $C_4$-symmetric insulator that breaks $M_x$ and $M_y$ in the topological phase. It has quantized corner charges $\pm \frac{\Delta}{2}$ but not quantized edge polarizations $\frac{\Delta}{2} + \Delta$, in a $C_4$ symmetric pattern.

which takes the values of $e^{i2\pi q_{xy}} = \pm 1$ in the trivial or topological quadrupole phases, respectively. This corresponds to quantized values of the quadrupole of

$$q_{xy} = \begin{cases} 0, & \text{if trivial} \\ \frac{1}{2}, & \text{if nontrivial}. \end{cases}$$

This index is independent of the choice of $C_4$ rotation operator, provided that the same operator is used at both $\Gamma$ and $\mathbf{M}$. For example, for the choice of $\hat{r}_4$ of (2.163), which obeys $\hat{r}_4^4 = -\tau_0 \otimes \tau_0$, its eigenvalues are $e^{\pm i\pi/4}$, $e^{\pm i3\pi/4}$, and the rotation eigenvalues in the trivial and topological quadrupole phases of (2.156) under $C_4$ symmetry are schematically shown in Fig. 2.33.

In $C_4$ symmetry-preserving transitions, $h^q(\mathbf{k})$ closes the bulk-energy gap at $\Gamma$, $X$, $Y$, or $M$, as indicated by the dots in Fig. 2.30. At these transitions, the rotation eigenvalues of the occupied energy bands change from the configuration in Fig. 2.33(b) to those in either Fig. 2.33(c) or Fig. 2.33(d).

We finally point out that, since $C_4$ symmetry does not protect the Wannier-sector polarizations, the quantization of the edge polarizations is not guaranteed in the presence of $C_4$ symmetry. For example, if $C_4$-symmetric perturbations having hopping terms between nearest-neighbor unit cells are added, the observables of the Hamiltonian could be modified as schematically shown in Fig. 2.34. Even though the edge polarizations are not quantized, (i) the corner charge remains quantized, and (ii) the relation between edge polarizations and corner charge still implies the existence of a quantized quadrupole moment, on top of which edge dipoles of magnitude $\Delta$ are overlapped in a $C_4$-symmetric pattern (see Sec. 2.2.4).

**Phase transitions in the quadrupole insulator**

The closing of either the energy gap or the Wannier gap is a property dictated by the bulk band parameters. In this section, we describe how the phase transitions in $h^q(\mathbf{k})$ manifest at the boundaries. In the following description, we set $\lambda_x = \lambda_y = 1$ for simplicity.
We start with the $C_4$, $M_x$, and $M_y$-symmetric transitions with full open boundaries. The energy bands for this system as a function of the parameter $\gamma = \gamma_x = \gamma_y$ are shown in Fig. 2.35(a). In the topological phase, the red lines denote the corner-localized, fourfold-degenerate modes, which are characteristic of the topological quadrupole phase, as seen in Fig. 2.35(b). During the transition, the bulk energy gap closes and the corner-localized states hybridize and fuse into the bulk and are no longer present in the trivial phase.

If we now drive the transition by varying $\gamma_y$ while keeping $|\gamma_x| < 1$, as in Fig. 2.35(c), only the energy gap of the edge parallel to $y$ closes. Consequently, as the transition is approached, the four corner modes hybridize in pairs along the edge parallel to $y$, as seen in Fig. 2.35(d). Recall that this phase transition is associated with a closing of the Wannier gap at $\nu_{y}(k_y = \pi) = \frac{1}{2}$ when the system has periodic boundary conditions (second column, first row, of Fig. 2.28). Hence, we conclude that a gap closing of the Wannier bands results in an energy gap closing in the 1D $x$-edge Hamiltonian. This relation between the bulk property of Wannier gap closing and the energy gap closing of the edge can be inferred from the adiabatic mapping connecting the Wannier bands to the Hamiltonian of the edge as detailed in Sec. 2.4.2.

Indeed, one can verify that the energy gap closing occurs along the $x$-edge by repeating the calculation in (c), but for a quadrupole insulator with periodic boundaries along $x$. This is shown in Fig. 2.36(a). In contrast to what happens in Fig. 2.35(c), the energy bands in Fig. 2.36(a) do not close the gap. In this setup, in which boundaries along $x$ ($y$) are closed (open), this transition can be visualized by plotting the Wannier bands $\nu_{y}^{j}$, for $j \in 1 \ldots 2N_y$, as a function of the parameter $\gamma_y$. This is shown in Fig. 2.36(b). The red line in this figure indicates the twofold Wannier-degenerate states that are localized at the two opposite $y$-edges, having Wannier value of $\frac{1}{2}$. These states are characteristic of the quadrupole phase and are responsible for the quantized edge polarizations (see Sec. 2.6.4). Analogous to the corner-localized modes in the energy plots, the edge-localized modes in the Wannier plots hybridize as the Wannier gap closes, and fuse into the bulk outside of the quadrupole phase. Physically, this plot illustrates that (even in the absence of corners) the edge polarizations are clear signatures that persist only as long as the bulk is in the quadrupole topological phase. The mapping described in Sec. 2.4.2 that adiabatically maps the Wannier bands of Fig. 2.36(b) to the edge energies in Fig. 2.35(c) is consistent with this phenomenology.

In the phase diagram in Fig. 2.30 for the quadrupole topological phases of $h\hat{q}(\mathbf{k})$, the blue and red lines indicate the edges at which the energy bands close for $M_x$- and $M_y$-preserving phase transitions, and the black dots indicate the points of the BZ at which the bulk energy bands close for $C_4$-preserving phase transitions.

2Although a bulk transition implies closing the edge energy gap, the contrary is not true, i.e., a closing of the edge energy gap as a result of a phase transition of the edge does not imply a transition in the bulk; in this latter case, the edge transition just causes the nontrivial edge at the boundary of the quadrupole to recede in order to exclude the outermost trivial edge that underwent the transition.
Figure 2.35: Two types of quadrupole phase transitions for Hamiltonian (2.156) with full open boundaries. For (a), (b) we have a $C_4$, $M_x$, and $M_y$ symmetric Hamiltonian. (a) Energy bands as a function of $\gamma = \gamma_x = \gamma_y$. (b) Probability density function of the zero-energy modes as the system approaches the transition with $C_4$, $M_x$, $M_y$ symmetric Hamiltonian, having $(\gamma_x, \gamma_y) = (0.75, 0.75)$. (c), (d) have $M_x$, and $M_y$ but not $C_4$ (c) energy bands as a function of $\gamma_y$ while fixing $\gamma_x = 0.5$. (d) Probability density function of the zero-energy modes as the system approaches the transition for a Hamiltonian having $(\gamma_x, \gamma_y) = (0.5, 0.75)$. In the simulations, there are $40 \times 40$ unit cells. For the purpose of illustration, unit cells in the range $N_{x,y} \in [5, 34]$ are in the topological quadrupole phase with $(\gamma_x, \gamma_y)$ as indicated. Unit cells outside of $N_{x,y} \in [5, 34]$ are in the trivial phase with $(\gamma_x, \gamma_y) = (2, 2)$. All unit cells have $\lambda_x = \lambda_y = 1$.

Figure 2.36: (a) Energy bands and (b) Wannier bands $\nu_j^{[y]}$, for $j \in 1 \ldots 2N_y$, with closed boundaries along $x$ and open along $y$ as a function of $\gamma_y$ while fixing $\gamma_x = 0.5$. In all plots $\lambda_x = \lambda_y = 1$. Red lines indicate the twofold-degenerate states with polarization $\frac{1}{2}$ localized at the open edges.

Let us make some final notes about the multi-critical nature of the bulk phase transition. We see that we only find a bulk phase transition in our phase diagram when $C_4$ symmetry is preserved. However, our phase diagram is implicitly assuming that both reflection symmetries are preserved since every point in the phase diagram has reflection symmetry by design. Hence, if we have both reflection symmetries and $C_4$ symmetry, we naturally have a bulk critical point where a transition occurs via a double Dirac point in momentum.
If we remove $C_4$ symmetry but preserve reflection symmetry, then we have already seen in detail that we will not generically have a bulk critical point separating the quadrupole phase from the trivial phase. Additionally, there is one more option we have not discussed which is to preserve $C_4$ symmetry, but break both reflection symmetries. We need to break both reflections because their product is proportional to the $C_2$ rotation operator, and hence must be preserved. This implies that both reflections are either preserved or both broken. In this scenario, there will still generically be a bulk gap closing when transitioning out of the quadrupole phase. However, the direct transition to a trivial insulator will be replaced by a two-step process with an intermediate phase separating the quadrupole insulator from the trivial insulator. As one tunes a single parameter, the quadrupole phase will first transition to a Chern insulator with a bulk gap closing at a single Dirac point. Then, as the parameter is further tuned, the Chern insulator will transition to the trivial phase through a second single Dirac point. Thus, breaking reflection symmetries will split the direct quadrupole-to-trivial transition into two single Dirac cone transitions with an intermediate Chern insulator phase. The Chern insulator phase is not compatible with reflection symmetry and hence does not appear in the phase diagram if reflection symmetry is preserved.

### 2.6.5 Dipole pumping

We now break the symmetries that protect the topological quadrupole phase by adding perturbations to the Hamiltonian (2.156). As a result, the quadrupole observables lose their quantization. We will see in particular that a new type of electronic pumping occurs, that of a dipole current.

Breaking the symmetries that quantize the quadrupole can occur in the following scenarios:

- Perturbation breaks $M_i$ and $C_2$ symmetries but keeps $M_j$. This quantizes $p_j^{\pm \nu_i}$ and the bulk dipole moment $p_j$ but does not quantize $p_i^{\pm \nu_j}$ nor the bulk dipole moment $p_i$. Here $i, j = x, y$ and $i \neq j$.

- Perturbation breaks $M_x$ and $M_y$ symmetries but keeps $C_2$ symmetries. This does not quantize $p_x^{\pm \nu_y}$ nor $p_y^{\pm \nu_x}$, but keeps the total bulk dipole moment quantized, e.g., $p = 0$.

We concentrate on the second scenario, because we are interested in pumping arising exclusively from the bulk quadrupole moment and not from dipole moment contributions. A perturbation that breaks both reflection symmetries while preserving $C_2$ is the one we have used in Eq. (2.166) to choose the “sign” of the quadrupole. The simplest and most illustrative pumping process consists of the adiabatic evolution of the
insulator in Eq. (2.166) parametrized by $t$ according to

\[
(\delta, \lambda, \gamma) = \begin{cases} 
(\cos(t), \sin(t), 0), & 0 < t \leq \pi \\
(\cos(t), 0, |\sin(t)|), & \pi < t \leq 2\pi,
\end{cases}
\]

(2.189)

where for simplicity we have chosen $\lambda_x = \lambda_y = \lambda$ and $\gamma_x = \gamma_y = \gamma$. During this process, the two-fold-degenerate energies in the bulk remain gapped for all times $t$: $\epsilon(k, t) = \pm \sqrt{1 + \sin^2(t)}$. Similarly, the energy gaps of the edges also remain gapped, which is crucial for adiabaticity. Figures 2.37(a) and 2.37(b) show the transport corresponding to the adiabatic evolution (2.189) during the first half of the cycle.

In Fig. 2.37(a) [Fig. 2.37(b)] boundaries are closed along $x$ ($y$) and open along $y$ ($x$), as schematically indicated by the cylinders. The plots track the Wannier values during the first half of the cycle during which all the inter-unit cell transport takes place. The dark blue lines correspond to Wannier eigenstates that extend over the bulk of the insulator. Each of the red, cyan, orange, and purple lines, on the other hand, correspond to one Wannier center whose wave function localizes at an edge of the insulator, as indicated by the corresponding lines on the cylinders. At $t = 0$, the insulator has the trivial Hamiltonian $\Gamma_0$. This is a momentum-independent Hamiltonian which represents an insulator in the trivial atomic limit, and therefore all its Wannier values are zero. As the system is adiabatically deformed, the on-site perturbation becomes
smaller and the hopping amplitudes increase. Two Wannier sectors appear, as well as Wannier eigenstates localized at the edges. At \( t = \pi/2 \), the reflection symmetries are restored, and we encounter the topological quadrupole phase of model (2.156), which has Wannier-sector polarization \( p^\nu_{ij} = \frac{1}{2} \) and consequent edge-localized polarizations of \( \frac{1}{2} \). The evolution continues, with hopping terms fading and on-site terms increasing magnitude, but with the opposite sign as in the range \( t \in [0, \pi/2) \). As we approach the end of the first half of the cycle, \( t \to \pi \), the system approaches the trivial phase, and \( p^\nu_{ij} \to 1 \mod 1 \). While the bulk Wannier states show no net transport after the half cycle, the edge-localized Wannier states show net transport of one electron from right to left by one unit cell on the upper boundary, and one from left to right by one unit cell on the lower boundary in Fig. 2.37(a). Figure 2.37(b) shows a similar pattern. The combined overall pattern of transport, however, is not that of a circulating current. Instead, it is consistent with a quadrupole pattern in which the bulk dipole remains fixed to zero, as shown in Fig. 2.37(c). During the second half of the cycle, \( \pi < t \leq 2\pi \), the Hamiltonian remains in the trivial atomic limit phase, and thus causes no electronic transport.

This adiabatic evolution is associated with a Berry flux and Chern number of the Wannier bands as calculated via

\[
\Delta q_{xy} = \int_0^{2\pi} d\tau \partial_\tau p^\nu_{ij} (\tau) = 1
\]  

(2.190)

for \( i, j = x, y \) and \( i \neq j \). In essence, this pumping process results in edge-localized Thouless pumping processes, associated with the changing edge polarizations due to the adiabatic evolution of the bulk quadrupole moment. During a full cycle there is quantized transport captured by the winding of the Wannier-sector polarizations (2.190), as shown numerically in Fig. 2.37(d) (the Wannier-sector polarization winds completely in the range \( t \in [0, \pi) \) because the Berry flux for \( t \in [\pi, 2\pi) \) is zero, since the Hamiltonian remains in the atomic-limit phase during this second half of the cycle).

The pumping process detailed above provides us with a family of Hamiltonians which, we claim, have quadrupole moments that range from 0 to 1. To confirm this, we track the corner charge and the edge polarizations during the entire cycle. The prescription for the calculation of the edge polarization is shown in Sec. 2.5. Figure 2.38 shows a plot of the instantaneous corner charge as well as the instantaneous edge polarization (we find that the magnitudes of the edge polarizations along all edges are equal). The edge polarizations are calculated by integrating the contributions to tangential polarization up to the middle of
the crystal, i.e., as

\[ p_{\text{edge}}^{-y} = \sum_{R_y=1}^{N_y} p_x(R_y), \quad p_{\text{edge}}^{+y} = \sum_{R_y=\frac{N_y}{2}+1}^{N_y} p_x(R_y), \]  

(2.191)

where \( p_x(R_y) \) is given by Eq. (2.126), and similarly for \( p_{\text{edge}}^{\pm x} \). The corner charges are calculated by integrating the charge density over a quadrant of the crystal, i.e., as

\[ Q_{\text{corner}}^{-x,-y} = \sum_{R_x=1}^{N_x} \sum_{R_y=1}^{N_y} \rho(R), \]  

(2.192)

where \( \rho(R) \) is the charge density over occupied states. A similar calculation follows for the other three corner charges in \( Q_{\text{corner}}^{\pm x, \pm y} \). The edge polarizations and the corner charges are the same, in agreement with (2.128), over the entire range of the pumping process. The bulk polarization remains zero during this process since \( C_2 \) symmetry is always preserved.

When calculating the overall edge polarization, following the prescription of Sec. 2.5, there is a subtlety. We find that there are two contributions that can be differentiated: one contribution is captured by the edge-localized eigenstates of the Wilson loop with open boundaries in one direction, which we call “topological”; the other, “non-topological” contribution, comes from eigenstates of the Wilson loop distributed over the bulk. These separate contributions are shown in Fig. 2.39(a). Numerically, the topological contribution is easily discriminated because its Wannier value is situated within the Wannier gap for \( t \in (0, \pi) \) [see Figs. 2.37(a) and 2.37(b)]. At \( t = 0, \pi \), on the other hand, all Wannier values vanish. We find that the Wannier-sector polarization (2.143) reflects the values of the topological term, as shown in Fig. 2.39(b), but does not capture the non-topological contribution. Hence, the Wannier-sector polarizations, i.e., the
polarization of the effective edge Hamiltonian should be treated as a symmetry protected topological invariant and not as a quantitative measure of the exact edge polarization when the symmetries are relaxed. We conjecture that this is because the effective edge Hamiltonian is only adiabatically connected to the physical edge Hamiltonian [66], thus, only topological properties are necessarily preserved. Importantly, the total edge polarizations and corner charges are all quantized to 0 or $\frac{1}{2}$ in the trivial or topological symmetry-protected quadrupole phases, respectively, and the non-topological contribution to edge polarization vanishes in the presence of the quantizing symmetries. Hence, although the Wannier-sector polarization does not describe the precise value of the edge polarization and corner charge when there is a bulk contribution to the edge polarization, it does correctly describe the topological properties of the quadrupole. Aside from providing the correct quantized values of the corner charge and edge polarization in the SPT phases, the quantization of dipole pumping is also correctly given by Eq. (2.190).

Opening the boundaries: Let us now elaborate on the pumping process from the point of view of the corner charges. The pattern of electronic current shown in Fig. 2.37(c) suggests that charge flows from one pair of opposite corners to the other pair. A direct calculation of the energy bands for this type of adiabatic pumping when boundaries along both $x$ and $y$ are open should reflect this pattern. Since it will become useful, let us do this by using an alternative parametrization of the pumping process which varies continuously over the entire adiabatic cycle [as opposed to pumping (2.189), which is continuous piecewise]. It is given by

$$h^q_{\text{pump}}(k,t) = [-m \cos(t) + 1](\Gamma^4 + \Gamma^2) - m \sin(t) \Gamma^0$$
$$+ \cos(k_x) \Gamma^4 + \sin(k_x) \Gamma^3 + \cos(k_y) \Gamma^2 + \sin(k_y) \Gamma^1.$$  (2.193)
Figure 2.40: Adiabatic pumping (2.193) with open boundaries in both directions. $t$ is the pumping adiabatic parameter. (a) Energy spectrum. Green (red) lines are twofold degenerate and have corresponding modes that localize at opposite corners. (b) Corner charge during pumping. Open blue (solid red) circles represent a corner charge of $+\frac{e}{2}$ ($-\frac{e}{2}$) at the beginning and end points of the pumping process. Charge inversion amounts to pumping a quantum of dipole moment.

The pumping process (2.193) maintains $C_2$ symmetry, with $\hat{r}_2 = -i\tau_0 \otimes \tau_2$, at all values of the adiabatic parameter $t \in [0, 2\pi)$, which locks the polarization to zero. For $0 < m < 2$ ($-2 < m < 0$), the insulator is in the quadrupole (trivial) phase at $t = 0$ and in the trivial (quadrupole) phase at $t = \pi$, while for $|m| > 2$ there is no dipole pumping, as the insulator is in the trivial phase at both $t = 0, \pi$. Figure 2.40 shows the adiabatic evolution of this Hamiltonian with $m = 1$ and open boundaries along both directions. In Fig. 2.40(a), the bulk energies (marked in dark blue) are gapped. The energies that cross the bulk-energy gap (marked in red and green) are each twofold degenerate (i.e., there are a total of four gap-crossing states), and correspond to the corner-localized states. The two degenerate states localize at opposite corners. At half-filling, the result of pumping is to change the values of the charges at the corners by $e$, as seen in Fig. 2.40(b) so that the final quadrupole is equivalent to the original one upon a rotation by $90^\circ$. In Fig. 2.40(b), we start at a time $\epsilon$ and finish at $2\pi - \epsilon$, for $\epsilon \ll 1$, so that we clearly define the initial sign of the quadrupole by slightly deviating away from the perfectly symmetric SPT quadrupole phase.

Although the pumping (2.189) also reflects the characteristics we just described, the convenience of the parametrization (2.193) will become evident when we make a connection between dipole pumping processes and a new type of topological insulator in one higher spatial dimension in Sec. 2.6.6.

### 2.6.6 Topological Insulator with hinge-localized chiral modes

In Sec. 2.3.6 we saw that adiabatic charge pumping in 1D insulators by means of a changing dipole moment is characterized by the winding of the Wannier eigenvalues as a function of the adiabatic parameter. This winding is equivalent to a Chern number in the mixed momentum-adiabatic parameter space. If we rename the adiabatic parameter $t$ in the model with a torus parametrization to a new momentum variable, e.g.,
If we substitute $t \to k_z$ in Eq. (2.193), the resulting model is the Hamiltonian of a 3D insulator with a winding quadrupole invariant along $k_z$. Fig. 2.41(a) shows the dispersion of this insulator when boundaries are open along both $x$ and $y$, but closed along $z$. Notice that this is in essence the same plot as that in Fig. 2.40(a). The interpretation, however, is different. The corner-localized modes during the adiabatic pumping now map to edge localized modes that are chiral and carry current in a quadrupolar fashion when an electric field along $z$ is applied. A schematic of this insulator is shown in Fig. 2.41(b). These hinge-localized modes are protected by the Wannier-band Chern number

$$n_{yz}^{\nu_i} = \frac{1}{(2\pi)^2} \int_{BZ} \text{Tr} \left[ \tilde{F}_{y,z,k}^{\nu_i} \right] d^3k, \quad (2.194)$$

where

$$\tilde{F}_{j,k,k}^{\nu_i} = \partial_j \tilde{A}_{k,k}^{\nu_i} - \partial_k \tilde{A}_{j,k}^{\nu_i} + i[\tilde{A}_{j,k}^{\nu_i}, \tilde{A}_{k,k}^{\nu_i}], \quad (2.195)$$

for $i,j,k = x,y,z$ and $i \neq j \neq k$, is the Berry curvature over the Wannier bands $\nu_i$, and $\tilde{A}_{j,k}^{\nu_i}$ is the Berry connection of the $\nu_i$ Wannier sector, defined in (2.144). A plot of these Wannier bands is shown in Fig. 2.41(c). They are gapped and each of them carry a Chern number (instead of just a Berry phase like the 2D quadrupole model). Notice that we always have

$$n_{jk}^{\nu_i} = -n_{kj}^{\nu_i}. \quad (2.196)$$

From this analysis we conclude that 3D insulators have additional anisotropic topological indices that signal the presence of chiral, hinge-localized states parallel to $x$, $y$, or $z$. For example, in the insulator of Fig. 2.41, we have

$$n_{yz}^{\nu_i} = -n_{xz}^{\nu_i} = 1, \quad n_{xy}^{\nu_i} = 0. \quad (2.197)$$

In general, this type of cyclic relationship is kept. Thus, unlike the weak indices for polarization (2.104), which are each independent of each other, the Chern numbers $n_{jk}^{\nu_i}$ defined in (2.194) are related by similar constraints to (2.197), as otherwise the hinge-localized modes would give incompatible hinge current flows.
Figure 2.41: A crystalline insulator with chiral, hinge-localized modes that disperse in equal directions at opposed corners and opposite directions in adjacent ones. This insulator is in the same topological class as the pumping (2.193). Both can be identified via the map $t \rightarrow k_z$. (a) Energy dispersion for a system with open boundaries along $x$ and $y$ but closed boundaries along $z$. (b) Hinge-localized states. Arrows indicate direction of dispersion in the presence of an electric field along $z$. (c) Wannier bands, each having a non-zero Chern number defined in (2.194). (d) Illustration of the compatibility relationship between Chern invariants (2.197). Circles indicate direction of chiral currents compatible with the hinge currents of (b).

See Fig. 2.41(d) for an illustration of the compatibility conditions. While the lateral surfaces have chiral currents described by the first Eq. in (2.197), the upper and lower surfaces have currents in a quadrupole pattern.

### 2.7 Bulk octupole moment in 3D crystals

The natural extension of the quadrupole moment in 2D is the octupole moment in 3D. In this section, we discuss in detail the calculation of the quantized octupole moment and describe a simple model that realizes it. We discuss both the SPT phase with quantized boundary signatures and an adiabatic pumping process. In particular, for the latter, we will see that an adiabatic cycle can pump a quantum of quadrupole moment.

#### 2.7.1 Simple model with quantized octupole moment in 3D

In order to have a well-defined octupole moment in the bulk of a 3D insulator, the bulk quadrupole and bulk dipole moments must vanish. Additionally, we require that no Wannier flow exists for Wannier centers along any direction, so as to avoid strong $\mathbb{Z}_2$ insulators and weak topological insulators with layered Chern
or $\mathbb{Z}_2$ QSH invariants that would result in metallic boundaries. Using these constraints, we can find a simple model for an octupole insulator as shown in Fig. 2.42. It has Bloch Hamiltonian

$$h_0^2(k) = \lambda_y \sin(k_y) \Gamma^1 + [\gamma_y + \lambda_y \cos(k_y)]\Gamma^2 + \lambda_x \sin(k_x) \Gamma^3 + [\gamma_x + \lambda_x \cos(k_x)]\Gamma^4 + \lambda_z \sin(k_z) \Gamma^5 + [\gamma_z + \lambda_z \cos(k_z)]\Gamma^6 + \delta \Gamma^6,$$

(2.198)

where $\Gamma^{ni} = \sigma_3 \otimes \Gamma^i$ for $i = 0, 1, 2, 3$, $\Gamma^4 = \sigma_1 \otimes I_{4 \times 4}$, $\Gamma^5 = \sigma_2 \otimes I_{4 \times 4}$, and $\Gamma^6 = i \Gamma^0 \Gamma^1 \Gamma^2 \Gamma^3 \Gamma^4 \Gamma^5$. Here, the internal degrees of freedom follow the numbering in Fig. 2.42. When $|\lambda_i| > |\gamma_i|$ for all $i = x, y, z$ this system is an insulator at half-filling with four occupied bands and a quantized octupole moment $o_{xyz} = \frac{1}{2}$. For $\delta = 0$, this Hamiltonian has reflection symmetries $M_{x,y,z}$ (up to a gauge transformation), with operators

$$\hat{M}_x = \tau_0 \otimes \tau_1 \otimes \tau_3, \quad \hat{M}_y = \tau_0 \otimes \tau_1 \otimes \tau_1, \quad \hat{M}_z = \tau_1 \otimes \tau_3 \otimes \tau_0,$$

(2.199)

which obey $\{\hat{M}_i, \hat{M}_j\} = 0$ for $i, j = x, y, z$ and $i \neq j$. The octupole moment $o_{xyz}$ is odd under each of these symmetries. In the continuum theory, this admits only the solution $o_{xyz} = 0$, but the ambiguity in the position of the electrons due to the introduction of the lattice (see Sec. 2.3.1) also allows the solution $o_{xyz} = \frac{1}{2}$ mod 1. In addition, these symmetries quantize $p_x, p_y, p_z, q_{xy}, q_{xz}, q_{yz}$, all of which must vanish for $o_{xyz}$ to be well-defined.

One signature of the topological octupole moment is the existence of fractional half charges localized on the corners of a cubic sample. Indeed, the nontrivial quantized octupole phase of this model has corner-localized mid-gap modes. We add an infinitesimal $\delta$ in the Hamiltonian that breaks the cubic symmetry of

![Figure 2.42: Lattice model of an octupole insulator with Bloch Hamiltonian (2.198).](image)
Figure 2.43: Electronic charge density of the octupole insulator with open boundaries. Corners have a charge of $\pm \frac{e}{2}$ relative to the background charge.

the crystal down to tetrahedral symmetry. This splits the degeneracy of the zero modes, hence fixing the sign of the octupole moment. A plot of the charge density for this crystal is shown in Fig. 2.43.

The four-dimensional subspace of occupied energy bands in the Hamiltonian (2.198) has reflection eigenvalues $\{-1, -1, +1, +1\}$ at all high-symmetry points. Consequently, the Wannier centers of the Wilson loop $W_{z,k}$ come in pairs $\{\pm \nu^1_z(k_\perp), \pm \nu^2_z(k_\perp)\}$, where $k_\perp = (k_x, k_y)$ (see Table 2.3). In the 3D BZ of Hamiltonian (2.198), the spectrum of the Wilson loop $W_{z,k}$ yields two, twofold-degenerate Wannier bands separated by a Wannier gap, i.e., $\nu^1_z(k_\perp) = \nu^2_z(k_\perp)$, as seen in Fig. 2.44. Since an octupole is made from two quadrupoles we want to show that each of these two-band Wannier sectors has a topological quadrupole moment. We now show how to determine this quadrupole moment.

### 2.7.2 Hierarchical topological structure of the Wannier bands

Microscopically, a bulk octupole can be thought of as arising from two spatially separated quadrupoles with opposite sign. Thus, since a quadrupole insulator requires two occupied bands, an octupole insulator requires a minimum of four occupied bands. Our model (2.198) is then a minimum model with octupole moment. To reveal its topological structure, we begin the analysis by performing a Wilson loop along the $z$ direction,

$$W_{z,k} \left| \nu^j_z, k \right\rangle = e^{i2\pi \nu^j_z(k_\perp)} \left| \nu^j_z, k \right\rangle,$$

where $k_\perp = (k_x, k_y)$. The Wilson loop along $z$ is represented by a $4 \times 4$ matrix, which has eigenstates $|\nu^j_z, k\rangle$ for $j = 1, 2, 3, 4$. In an octupole phase, the Wilson loop splits the four occupied energy bands into two Wannier sectors $\nu^\pm_z(k_\perp)$, separated by a Wannier gap. The existence of the Wannier gap is protected by the non-commutation of reflections operators (2.199). Each of the two sectors, $\nu^\pm_z$, has opposite
Figure 2.44: Schematic of the procedure to determine the topology of an octupole moment. A Wilson loop along $z$ over the 3D BZ (purple cube) divides it into two sectors, according to its Wannier value $\nu_z^\pm$ (red and light blue plots over the cube). Each sector has two bands (represented by the red and blue squares) and has quadrupole topology. This can be verified by calculating Wilson loops along $y$ over each sector, which renders two Wannier sectors $\eta_y^\pm$ (red or blue pair of symmetric lines), each of them having a Berry phase of 0 or $\pi$ in its Wilson loop along $x$ in the $|\lambda_i| < |\gamma_i|$ (for all $i$) or $|\lambda_i| > |\gamma_i|$ (for all $i$) regime, respectively.

topological quadrupole moment. The Wannier bands $\nu_z^\pm$ for the minimal octupole insulator with Hamiltonian in Eq. (2.198) are shown in red and light blue in Fig. 2.44.

In order to determine the quadrupole moment of each of the sectors $\nu_z^\pm$, we proceed similarly to Sec. 2.6 for either $\nu_z^+$ or $\nu_z^-$. Concretely, let us first re-write Eq. (2.200) as

$$W_{z,k} \left| \nu_z^{\pm,j} \right\rangle = e^{i 2 \pi \nu_z^\pm (k_z)} \left| \nu_z^{\pm,j} \right\rangle ,$$

for $j = 1, 2$. Without loss of generality, we choose the sector $\nu_z^+$ and construct the Wannier states

$$\left| w_{z,k}^{+,j} \right\rangle = \sum_{n=1}^{N_{occ}} |u_{n,k}^{\nu_z,k} \rangle |\nu_z^{+,j} \rangle^n ,$$

for $j = 1, 2$. Here, the superscript $+z$ is short for the Wannier sector $\nu_z^+$. We use this basis to calculate the nested Wilson loop along $y$,

$$W_{y,k}^{+,j} = \left| w_{z,k+N_y,\Delta_{k_y}}^{+,j} \right\rangle \left( w_{z,k+(N_y-1)\Delta_{k_y}}^{+,r} \left| w_{z,k+(N_y-1)\Delta_{k_y}}^{+,r} \right\rangle \cdots \left| w_{z,k+\Delta_{k_y}}^{+,s} \right\rangle \left| w_{z,k}^{+,j} \right\rangle ,$$

where $\Delta_{k_y} = (0, 2\pi/N_y, 0)$. Notice that, since $j, r, \ldots, s, j' = 1, 2$, this nested Wilson loop is non-Abelian. [This Wilson loop was defined in Eq. (2.138) for 2D crystals, but we reproduce it here in its obvious extension.
to 3D). We then diagonalize the nested Wilson loop (2.203),

$$\hat{W}_{y,k}^{+} \ket{\eta_{y,k}^{+,\pm}} = e^{i2\pi \eta_{y}^{+}(k_x)} \ket{\eta_{y,k}^{+,\pm}},$$ (2.204)

which resolves the Wannier sector $\nu_{z}^{+}$ into single Wannier bands $\eta_{y}^{+}(k_x)$ separated by a Wannier gap (red lines on axes $\eta_y$ in Fig. 2.44). This Wannier gap is also protected by the non-commutation of (2.199). The quadrupole topology of the Wannier sector $\nu_{z}^{+}$ manifests in that each of the sectors $\eta_{y}^{\pm}$ has a quantized dipole moment, indicated by a Berry phase of 0 or $\pi$. For example, let us choose the sector $\eta_{y}^{+}$, to define the Wannier basis

$$\ket{w_{y,k}^{+}} = \sum_{n=1}^{N_{occ}} |u_{n,k}^{y}|^{2} \ket{\eta_{y,k}^{+,+}}.$$ (2.205)

to then calculate a third Wilson loop

$$\hat{W}_{x,k}^{+} = \bra{w_{y,k+N_{y} \Delta k_{x}}^{+,+} w_{y,k+N_{y} \Delta k_{x}}^{+,+} \cdots w_{y,k+N_{y} \Delta k_{x}}^{+,+} w_{y,k}^{+}}.$$ (2.206)

This Wilson loop is associated with the Wannier-sector polarization

$$p_{x}^{+,+} = -\frac{i}{2\pi N_{y} N_{z}} \sum_{k_y,k_z} \text{Log} \left[ \hat{W}_{x,k}^{+,+} \right]$$ (2.207)

and which for our model takes the values

$$p_{x}^{+,+} = \begin{cases} 
\frac{1}{2}, & |\gamma_{i}| > |\lambda_{i}| \\
0, & |\gamma_{i}| < |\lambda_{i}| 
\end{cases}$$ (2.208)

for all $i$. From this, it follows that the topology of each original Wannier sector $\nu_{z}^{\pm}$ is that of a quadrupole, and the topology of the entire Hamiltonian is that of an octupole.

In this calculation, the order of the nested Wilson loops $W_{z} \rightarrow W_{y} \rightarrow W_{x}$ was arbitrary. The same results as in (2.208) are obtained for any order of Wilson loop nesting in a quantized octupole insulator, provided that the non-commuting quantizing symmetries are present.

### 2.7.3 Boundary signatures

Classically, the octupole moment manifests at the faces of a 3D material by the existence of surface-bound quadrupole moments (see Sec. 2.2). In this formulation, the connection between the bulk topology and the
boundary topology is given by the adiabatic map between the Wilson loops spectrum and the spectrum of the physical boundary Hamiltonians (see Sec. 2.4.2). Thus, in the formulation derived in Sec. 2.7.2 to characterize the bulk topology of an octupole insulator, we can make the identification

$$W_{z,k} = e^{-iH_{\text{surface}}(k)},$$

(2.209)

where $W_{z,k}$ is the Wilson loop along $z$ of Eq. (2.200), and $H_{\text{surface}}(k)$ has the same topology of the Hamiltonian at the surface of the insulator in the $xy$ plane (we can similarly assign Wilson loops along $x$ ($y$) to Hamiltonians on the surface $yz$ ($zx$)). Similarly, we can make the identification

$$\tilde{W}_{y,k}^{\pm} = e^{-iH_{\text{hinge}}(k)},$$

(2.210)

where $\tilde{W}_{y,k}^{\pm}$ is the nested Wilson loop defined in (2.203), and $H_{\text{hinge}}(k)$ has the same topological properties as the Hamiltonian at the one-dimensional boundaries of the 2D surface $xy$ of the material (i.e., we are now looking into the boundary of the boundary). Notice that in all levels of nesting of the Wilson loops, their Wannier bands remain gapped, which was a condition imposed to avoid boundary metallic modes. Since the Wannier Hamiltonians and edge Hamiltonians are adiabatically connected this implies that when the Wannier Hamiltonians are gapped, the corresponding boundary Hamiltonians are energy gapped.

### 2.7.4 Quadrupole pumping

Just as a varying dipole generates charge pumping, and a varying quadrupole generates dipole pumping (pumping of charge on the boundary), an adiabatic evolution of the octupole insulator which interpolates between the topological octupole phase and the trivial octupole phase pumps a quantum of quadrupole. This can be achieved by the Hamiltonian

$$h_{\text{pump}}^o(k, t) = (-m \cos(t) + 1)(\Gamma^{r2} + \Gamma^{r4} + \Gamma^{r6}) - m \sin(t)\Gamma^{r0}$$

$$+ (\sin(k_y)\Gamma^{r1} + \cos(k_y)\Gamma^{r2})$$

$$+ (\sin(k_x)\Gamma^{r3} + \cos(k_x)\Gamma^{r4})$$

$$+ (\sin(k_z)\Gamma^{r5} + \cos(k_z)\Gamma^{r6}),$$

(2.211)
for \( t \in [0, 2\pi) \), where \( t \) is the adiabatic parameter. The adiabatic cycle can be characterized by a topological invariant that captures the change in octupole moment:

\[
\Delta o_{xyz} = \int_0^{2\pi} d\tau \partial_\tau p_k^{\pm;\pm;\pm}(\tau) = 1 
\]

for \( i, j, k = x, y, z \) and \( i \neq j \neq k \), and where \( p_k^{\pm;\pm;\pm}(\tau) \) is defined as in Eq. (2.207) for the instantaneous Hamiltonian (2.211). This particular pumping process preserves the in-plane \( C_2 \) symmetries \((x, y, z) \rightarrow (x, -y, -z), (-x, y, -z) \rightarrow (x, y, -z), \) and \((x, y, z) \rightarrow (-x, -y, z)\) at all times \( t \in [0, 2\pi) \), but breaks the reflection symmetries and the overall inversion symmetry \((x, y, z) \rightarrow (-x, -y, -z)\), except at the SPT phase points at \( t = 0, \pi \). Breaking the reflection symmetries while preserving the in-plane symmetries allows transport only through the hinges, via surface dipole pumping processes. This occurs at all hinges, so that the octupole configuration is inverted as illustrated in Fig. 2.45. The overall effect amounts to a pumping of a quantum of quadrupole through the 3D bulk.

Figure 2.45: Initial (left) and final (right) octupole insulators as the result of adiabatic pumping by the Hamiltonian (2.211). Blue (red) dots represent corner-localized charges of \( \pm \frac{e}{2} \), respectively. A quantum of quadrupole moment is pumped in the process.

### 2.8 Summary

In this Chapter, we have systematically addressed the question of whether insulators can give rise to quantized higher electric multipole moments. Starting from the derivation of observables in a classical, continuum electromagnetic setting, we established the physical signatures of these moments and discussed how the definitions could be generalized for an extended quantum mechanical system in a lattice.

In the crystalline, quantum mechanical theory, we found that the same macroscopic relations as in the classical continuum theory are maintained.

We have also shown that the topological structure of these SPT phases is hierarchical in a way that reflects the relationship between a bulk multipole moment and the lower moments realized on the boundary.
For example, the subspace of occupied bands in a quadrupole has two sectors, each having nontrivial dipole topology, while the subspace of occupied bands of an octupole moment has two sectors, each having non-trivial quadrupole topology. Through this hierarchical topological classification, we were able to construct topological invariants that characterize the bulk SPT phases. One can also break the protecting symmetries to generate non-quantized multipole moments, and in such a scenario one can develop protocols by which the system is driven in adiabatic cycles so that the multipole moment changes by a quantized amount and topological pumping occurs.

Such topological pumping processes can also be used to construct topological insulators in one dimension higher where the adiabatic pumping parameter is interpreted as an additional momentum parameter. We provided an example of this in an adiabatic pumping process where the quadrupole moment changes by an integer and gives rise to an associated 3D insulator with chiral states on the hinges of the material.
Chapter 3

Majorana bound states at topological defects in crystalline superconductors

3.1 Introduction

In Chapter 3, we learned that zero-energy modes exist at the corners of quadrupole or octupole topological insulators. This suggests that certain 2D topological crystalline superconductors could harbor corner-localized Majorana bound states (MBS). In this Chapter, we explore this possibility. Furthermore, we focus on the possibility that MBS may be trapped at topological defects in these crystals\(^2\).

MBS are expected to be present in one and two-dimensional \(p\)-wave superconductors \([93, 94, 95]\) as boundary or vortex excitations, and in non-Abelian Quantum Hall states \([96, 97, 98]\) as Ising quasi-particle excitations. More recently, with the discovery of topological insulators (TI) \([22, 99, 100, 101, 102, 103, 104, 105]\), MBS are predicted to exist in heterostructures such as superconductor (SC) - ferromagnet (FM) interfaces in proximity with quantum spin Hall insulators \([106, 107, 108, 109, 110]\) and strong spin-orbit coupled semiconductors \([111, 112, 113]\).

For the latter cases of heterostructures devices, the MBS are trapped on non-dynamical defects such as domain walls. These defect MBS are conceptually distinct from quantum deconfined Ising anyons in topological phases \([114, 115, 116]\) like the Pfaffian quantum Hall state \([96, 97, 98]\), the chiral \(p_x + ip_y\) superconductor \([94, 95, 55]\), or the Kitaev honeycomb model \([56]\). The difference is that they are not fundamental excitations that rely on the existence non-Abelian topological order of a quantum system, but are extrinsic semiclassical objects associated to a point defect involving a topological winding of a set of order parameters \([117, 118]\). For example, the existence of MBS at TI-SC-FM heterostructures is a consequence of a topological order parameter texture formed from configurations of the band inversion TI gap, the proximity-induced pairing gap, and the gap due to magnetic order. To prevent the MBS from escaping the proximity interfaces in a heterostructure are required to be continuous, which may not be easy to achieve in reality. In this Chapter, we explore the theoretical possibility of manifesting defect MBS in homogeneous time reversal breaking superconductors that do not require strong spin-orbit coupling or extrinsic magnetic

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Defects like a quantum vortex in a chiral superconductor [119, 94, 95, 55] or a dislocation when discrete translation symmetry is present in a weak topological phase [120, 118, 121, 122, 123, 124] can bind MBS when a Bogoliubov-de Gennes (BdG) quasi-particle encircling the defect picks up a $\pi$ Berry phase. A single defect MBS in the BdG description has exactly zero energy pinned by particle-hole (or charge conjugation) symmetry. Its existence (or in general the MBS number parity) was shown in Ref. [118] to be topologically determined by a Chern-Simons $\mathbb{Z}_2$-invariant [118]

$$\Theta = \frac{1}{4\pi^2} \int_{BZ \times S^1} \text{Tr} \left( \mathcal{A} \wedge d\mathcal{A} + \frac{2}{3} \mathcal{A} \wedge \mathcal{A} \wedge \mathcal{A} \right)$$

modulo 2, where $\mathcal{A}_m^u(k, s) = \langle u_m(k, s) | du_n(k, s) \rangle$ is the Berry connection of occupied BdG states $|u_m(k, s)\rangle$ with crystal momentum $k$ in the Brillouin zone (BZ) and at position $s$ along a real-space circle $S^1$ around the defect. The index in Eq. 3.1 captures the interplay between the topology of the bulk BdG Hamiltonian and the structure of the classical defect. For example, the number parities of MBS at a quantum vortex and a dislocation are respectively given by

$$\Theta_{\text{vortex}} = \frac{1}{2\pi} \frac{\Phi}{\phi_0} C h, \quad \Theta_{\text{dislocation}} = \frac{1}{2\pi} \mathbf{B} \cdot \mathbf{G}_\nu$$

modulo 2, where $Ch$ is the Chern number that corresponds to edge chirality of the SC, and the weak invariant $G_\nu$ characterizes a 2D topological array of weakly coupled SC wires. These quantities are bulk topological information, while the number of flux quanta $\Phi/\phi_0$ and dislocation Burgers’ vector $\mathbf{B}$ are classical defect quantities. We see that the index depends on both, i.e., topological information about the electronic structure and the defect itself.

While the topological index in Eq. 3.1 completely characterizes the number parity of MBS at any arbitrary point defects in two-dimensional SC, it is not easily applicable to a real material as it requires a continuous diagonalization $u_m(k, s)$ of a spatially modulated, and sometimes complicated, Hamiltonian. The main objective of this Chapter is to generalize Eq. 3.2 into a topological index that applies to a more general class of crystalline defects and only involves detail independent quantities that are in principle experimentally measurable. The special case for disclinations in $C_4$ symmetric TCS, including all layered perovskite structures, was discussed in Ref. [124]. Here we extend the theorem to all discrete rotation symmetric SC
systems, and the index that counts MBS number parity takes the following general form:

\[
\Theta = \frac{1}{2\pi} \mathbf{T} \cdot \mathbf{G}_\nu + \frac{\Omega}{2\pi} (Ch + \text{rotation invariants})
\] (3.3)

modulo 2, where \((\mathbf{T}, \Omega)\) are discrete translation and rotation holonomic quantities of a lattice disclination that can be determined experimentally, for example, by neutron scattering, the Chern number \(Ch\) and weak invariant \(G_\nu\) correspond to protected gapless edge modes which in theory carry signatures detectable by ARPES or transport, and the rotation invariants are combinations of the rotation eigenvalues of the BdG quasi-particles.

### 3.1.1 Outline

Section 3.2 begins with a brief review of the classification of two-dimensional BCS superconductors in the BdG framework. The notion of equivariant stable classification is introduced and is followed by the definitions of integral rotation invariants in a TCS using rotation spectra at fixed points in the Brillouin zone. The constraints these invariants impose on the Chern and weak invariants are also discussed.

Section 3.3, proves that the Chern number and rotation invariants completely classify the topology of discrete-rotation symmetric TCS. This section also describes the algebraic structure of the classification, which reveals that a set of primitive models, or *generators*, can always be constructed to serve as fundamental building blocks of the different topological classes because any arbitrary Hamiltonian is stably topologically equivalent to certain copies of them. Explicit sets of such primitive generator Hamiltonians are constructed for each symmetry, and their classification is shown. These primitive models are either chiral \(p_x + ip_y\) superconductors or rotation symmetric arrays of 2-dimensional \(p\)-wave wires.

Section 3.4 provides a review of the classification of lattice disclinations in terms of their holonomies. Disclination holonomies are composed of a rotation and a translation piece, both of which enter the index theorems for the parity of MBS in \(C_4\) and \(C_2\) symmetric TCS, while only the rotation part enters the index for \(C_6\) and \(C_3\) symmetric TCS.

Section 3.5 begins by stating the general form of the topological index as a bilinear function of the disclination holonomic quantities (Frank angle and the effective Burgers’ vector) and topological Chern and rotation invariants. The index determines the parity of the number of MBS at a dislocation-disclination-flux composite of an arbitrary TCS described by a BdG Hamiltonian. By numerical and analytical exact diagonalization of the primitive model Hamiltonians at various disclinations and flux configurations, Majorana bound states are revealed and appear as localized zero energy BdG eigenstates. These explicit results enable
us to algebraically prove index theorems in the form of Eq. 3.3 for all lattice rotation symmetries. A detailed description of the lattice configurations used in the numerical simulations and some of the detailed numerical results are given in Ref. [37]. In Section 3.6 the indices of the preceding section are used to predict the existence of MBS in Strontium Ruthenate Sr$_2$RuO$_4$. A corollary result that we find is that even in the absence of disclinations, MBS will be manifested as corner states at open boundaries of the materials. Finally, in section 3.7 we briefly mention a few possible extensions of our work and consider an extrapolation of this study to a model constructed from a 3D array of p-wave wires, in which corner states are found. We then present our conclusions.

3.2 Topological invariants and stable classifications

Consider superconductors described by a BCS mean-field Hamiltonian in two dimensions

$$H = \int \frac{d^2 k}{(2\pi)^2} \xi_k^\dagger H_{BdG}(k) \xi_k$$

where $\xi_k = (c_\alpha(k), c_\alpha^\dagger(-k))$ is the Nambu basis. The Bogoliubov-de-Gennes Hamiltonian $H_{BdG}(k)$ is a band Hamiltonian on a toric Brillouin zone that obeys particle-hole (PH) symmetry

$$\Xi H_{BdG}(k) \Xi^\dagger = -H_{BdG}(-k)$$

where the PH operator $\Xi$ is anti-unitary and obeys $\Xi^2 = +1$, which corresponds to class D in the Altland and Zirnbauer 10-fold classification [125, 126, 127]. In our convention, $\Xi$ is a product of a unitary operator and the complex conjugation operator. We focus our study on systems having a finite excitation gap, and additionally a discrete symmetry $Pn = C_n \rtimes L$, where $C_n = \mathbb{Z}_n$ is an $n$-fold rotation point group and $L = \mathbb{Z}^2$ is the two-dimensional discrete translation group. We will not consider reflection symmetries in this work. Since we are dealing with fermionic systems, the rotation group is lifted to its double cover $\tilde{C}_n = \mathbb{Z}_{2n}$ so that a $360^\circ$ rotation produces a minus sign. The discrete rotation operator $\hat{r}_n$ that generates the group obeys $\hat{r}_n^2 = -1$. Additionally, $\hat{r}_n$ obeys

$$\hat{r}_n^\dagger \hat{H}_{BdG}(R_n k) \hat{r}_n = \hat{H}_{BdG}(k)$$

where $R_n$ is the $n$-fold rotation matrix acting on the momentum vector $k$. The rotation operator in an electronic system is charge conserving thus, in the BdG formalism, the rotation operator commutes with the
particle-hole symmetry operator

$$\Xi r_n \Xi^{-1} = \hat{r}_n.$$  \hspace{1cm} (3.7)

Before we introduce a classification scheme for the set of superconductor Hamiltonians we need to provide a definition of equivalence for two Hamiltonians. First, let us explicitly define the (direct) addition operation for two Hamiltonians. Given two superconductors with Hamiltonians $H_1$ and $H_2$, rotation representations $\hat{r}_1$ and $\hat{r}_2$, and PH operators $\Xi_1$ and $\Xi_2$, it is possible to combine them together into a composite superconductor with Hamiltonian

$$H_1 \oplus H_2 = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix},$$

and with symmetry operators represented accordingly by $\hat{r} = \hat{r}_1 \oplus \hat{r}_2$ and $\Xi = \Xi_1 \oplus \Xi_2$. Physically, this sum operation represents stacking together the two systems while keeping them decoupled. Two Hamiltonians $H_0(k), H_1(k)$ are said to be strictly equivalent if there is a continuous deformation $H_s(k)$ parameterized by $s$ for $0 \leq s \leq 1$ (with “endpoints” $H_0$ and $H_1$) so that (i) $H_s(k)$ remains gapped with no zero-energy eigenvalues for all $k$ and $s$, and (ii) $H_s(k)$ respects PH and the required spatial symmetries for all $s$. The physically relevant definition of equivalence is not the strict one, instead, we use the concept of stable equivalence\[127, 118\]. If two Hamiltonians are equivalent up to the (direct) addition trivial bands, i.e., if there are trivial, momentum-independent Hamiltonians $\mathcal{E}_0, \mathcal{E}_1$ (with their own PH and rotation representations) such that $H_0(k) \oplus \mathcal{E}_0$ is strictly equivalent to $H_1(k) \oplus \mathcal{E}_1$, then the Hamiltonians are said to be stably equivalent. Physically, $\mathcal{E}_{0,1}$ represent core or high energy atomic bands that are far away from the Fermi energy and are neglected in the Hamiltonians $H_{0,1}(k)$. They, however, could in principle be brought near the Fermi level and hybridize with the relevant bands during a deformation process. Subsequently, there are stably equivalent systems that are not strictly equivalent.

By identifying stably equivalent Hamiltonians, the set of equivalence classes forms a group under the operation of addition defined above; this is called the $K$-group \[127, 128\]. The classes of stably equivalent Hamiltonians $[H]$ form the elements of the group and each element represents a different topological class of Hamiltonians that cannot be adiabatically connected. The zero element of the $K$-group is the class of topologically trivial Hamiltonians, most simply represented by a system in the decoupled atomic limit in which electrons are bound to atoms on a lattice and cannot tunnel, and therefore have a BdG Hamiltonian and Bloch states that are momentum independent. To form a group each element must also have an inverse. In our case the additive inverse of an element is given by $[-H] = -[H]$ since $H(k) \oplus -H(k)$ can be smoothly
deformed into a constant Hamiltonian.

Now, after establishing what it means for two Hamiltonians to be equivalent, we need to find a set of topological invariants that will uniquely distinguish each element of the group. We find that for each rotation symmetry there is a different classification because each symmetry generates a different set of rotational topological invariants that distinguish the different elements of the $K$-group. Our classification also takes into account the two types of invariants whose existence is independent of the particular rotation symmetry, and in fact neither require rotation symmetry to be protected at all to be robust. These latter invariants are (i) the Chern invariant

$$
Ch = \frac{i}{2\pi} \int_{BZ} \text{Tr}(F) \in \mathbb{Z} \tag{3.9}
$$

where $F = dA + A \wedge A$ is the Berry curvature over the ‘occupied’ bands and $A^{\alpha\beta}(k) = \langle u^{\alpha}(k)|d\psi^{\beta}(k)\rangle$ is the Berry connection for band indices $\alpha, \beta$; and (ii) the two weak $\mathbb{Z}_2$-topological invariants

$$
\nu_i = \frac{i}{\pi} \int_{C_i} \text{Tr}(A) \mod 2 \tag{3.10}
$$

for $i = 1, 2$. Here, $C_i(s) = \pi \mathbf{b}_i + s\epsilon_{ij}\mathbf{b}_j$ is a closed path on the boundary of the Brillouin zone along the direction of the (unit normalized) reciprocal lattice vector $\epsilon_{ij}\mathbf{b}_j$ (see Fig. 3.1). These invariants are defined mod 2 because they can be changed by an even integer through a gauge transformation. They form a $\mathbb{Z}_2$-valued reciprocal lattice vector

$$
\mathbf{G}_\nu = 2\pi (\nu_1\mathbf{b}_1 + \nu_2\mathbf{b}_2) \tag{3.11}
$$

and are referred to as first-descendant invariants.

We note that there also exist second-descendant invariants $\mu(\Gamma_i)$; one for each of the four PH fixed
Figure 3.2: Brillouin zones for systems with (a) fourfold, (b) twofold, (c) sixfold, and (d) threefold rotation symmetries and their rotation fixed points. Shaded regions indicate the fundamental domain that generates the entire Brillouin zone upon rotation around the fixed point at the center of the Brillouin zones $\Gamma = (0, 0)$.

The momenta $\Gamma_i = \pi(m_1 \mathbf{b}_1 + m_2 \mathbf{b}_1)$, $m_j = 0, 1$. They are defined by

$$(-1)^{\mu(\Gamma_i)} = \frac{\text{Pf}[H(\Gamma_i)]}{\sqrt{\det[H(\Gamma_i)]}}$$  \hspace{1cm} (3.12)

where Pf means the pfaffian of the matrix in a choice of basis where the PH operator takes the form of the identity matrix multiplying complex conjugation $\Xi = K$. In this basis the Hamiltonian at each $\Gamma_i$ is antisymmetric $H(\Gamma_i) = -H(\Gamma_i)^T$ and the pfaffian is well-defined. The 2nd descendant invariants are not all independent and are restricted by the Chern and weak invariants:

$$\nu_1 = \mu(\pi \mathbf{b}_1) + \mu(\pi (\mathbf{b}_1 + \mathbf{b}_2)) \mod 2$$
$$\nu_2 = \mu(\pi \mathbf{b}_2) + \mu(\pi (\mathbf{b}_1 + \mathbf{b}_2)) \mod 2$$
$$Ch = \sum_{i=1}^{4} \mu(\Gamma_i) \mod 2.$$  \hspace{1cm} (3.13)

Thus, there is only one independent second-descendant invariant. However, this invariant does not aid the classification because it is unstable, i.e., it can be altered by the addition of trivial bands. Thus, while this is a topological invariant of an explicit Hamiltonian it does not contribute to the stable classification and so we will not discuss it further.

From our discussion so far we see that our 2D superconductors are classified by the Chern number and a vector of weak invariants which exist independent of rotation symmetry. Now we will provide the other necessary invariants to classify rotation invariant topological superconductors on a case-by-case basis. We proceed by defining the rotation invariants for each discrete rotation symmetry, and then we will examine the constraints that exist between these rotation-dependent invariants and the Chern and weak invariants.
3.2.1 Rotation eigenvalues and invariants

The Brillouin zones for $C_{2,3,4,6}$ symmetric Hamiltonians are shown in Fig. 3.2. Their periodicity implies that there are certain points $\Pi^{(n)}$ in momentum space that transform to themselves under some $n$-fold rotation $R_n$, that is, there exist fixed points at which

$$R_n \Pi^{(n)} = \Pi^{(n)}$$  \hspace{1cm} (3.14)

up to a reciprocal lattice vector. At these fixed points we have, from Eq. 3.6,

$$[\hat{r}_n, \hat{H}_{BdG}(\Pi^{(n)})] = 0.$$  \hspace{1cm} (3.15)

Thus, it is possible to label the states at the fixed points $\Pi^{(n)}$ by their rotation eigenvalues

$$\Pi_p^{(n)} = e^{i\pi(2p-1)/n}, \text{ for } p = 1, 2, \ldots, n.$$  \hspace{1cm} (3.16)

Let us denote $\#\Pi_p^{(n)}$ to be the number of occupied states with eigenvalues $\Pi_p^{(n)}$ at momentum fixed point $\Pi^{(n)}$. The key for the rotation invariant classification is that equivalent systems have the same set of numbers $\{\#\Pi_p^{(n)}\}$, though it does not matter in which order the occur energetically. This, however, does not suffice as full criteria for a classification, since the topological classes are not merely given by the sets of equivalent Hamiltonians, but rather by the sets of stably equivalent Hamiltonians, which are equivalent up to the addition of trivial bands. Since in the atomic limit trivial bands are momentum-independent, the numbers $\#\Pi_p^{(n)}$ at most fixed momenta are redundant for their classification as they are identical to that at the origin $\#\Gamma_p^{(n)}$. (Here $\Gamma = (0,0)$ is the center of the Brillouin zone, and therefore is a rotation fixed momentum under the full rotation symmetry.) Thus, topologically trivial BdG Hamiltonians are classified by representations of the rotation symmetry at a single fixed point, conventionally chosen to be $\Gamma$. Different representations of the rotation symmetry at the $\Gamma$-point can correspond to inequivalent atomic limits; however, this does not affect the stable classification as all atomic limits are topologically trivial.

Topologically non-trivial Hamiltonians are by definition not in the atomic limit so we must “quotient out” the atomic limits by taking the differences

$$[\Pi_p^{(n)}] = \#\Pi_p^{(n)} - \#\Gamma_p^{(n)}$$  \hspace{1cm} (3.17)

which are always integers. They can be non-trivial only when the Hamiltonian depends on momentum
because to be non-vanishing the eigenstates at \( k = 0 \) must behave differently under rotation than the ones at non-zero momentum. By taking the difference of rotation eigenvalues we are only retaining the non-trivial topological information and removing all information about trivial bands. The rotation invariants in Eq. 3.17 are therefore rotation symmetry protected topological signatures.

Before we move on to discuss each explicit rotation symmetry let us mention some general properties of the rotation eigenvalues. First, the commutativity between the PH and rotation operators relates the rotation eigenvalues of occupied and unoccupied bands. If the rotation eigenvalue of a state is \( \Pi_p^{(n)} \), the eigenvalue of the state related by PH symmetry is its complex conjugate \( \Pi_p^{(n)*} = \Pi_{n-p+1}^{(n)} \). Thus, \( \# \Pi_p^{(n)} \), the number of occupied bands with eigenvalue \( \Pi_p^{(n)} \), is also equal to the number of unoccupied states with eigenvalues \( \Pi_{n-p+1}^{(n)} \). This reduces the number of required invariants in the classification, as it makes some of them redundant due to the constraint

\[
\left[ \Pi_p^{(n)} \right]_{PH} = - \left[ \Pi_{n-p+1}^{(n)} \right]
\]

as will be seen shortly in a concrete example for the case of \( C_4 \)-symmetric systems.

Second, we briefly comment on the role of time reversal symmetry (TRS) on the rotation invariants. We have mentioned that all of our non-trivial topological models break TRS; this is not accidental, for if a system is time-reversal symmetric it obeys

\[
\Theta H(k) \Theta^{-1} = H(-k), \quad \Theta \hat{r}_n \Theta^{-1} = \hat{r}_n
\]

where \( \Theta \) is the anti-unitary time-reversal (TR) operator. This implies that if the rotation eigenvalue of a time-reversal symmetric state is \( \Pi_p^{(n)} \), then so must be its complex conjugate \( \Pi_p^{(n)*} = \Pi_{n-p+1}^{(n)} \). For the rotation invariants, this leads to the relation

\[
\left[ \Pi_p^{(n)} \right]_{TR} = \left[ \Pi_{n-p+1}^{(n)} \right]
\]

which is in contradiction with Eq. 3.18, unless the invariants are zero. Thus, any system that preserves TRS has trivial rotation invariants.

We also note that when the order of rotation \( n \) is even, there are two distinct rotation generators \( \pm \hat{r}_n \), both of which satisfy the fermionic requirement \( (\pm \hat{r}_n)^n = -1 \) since \( n \) is even. If we pick the other choice of rotation operator then the introduction of the extra sign changes the rotation invariants in a way that
depends on the order of the momentum fixed point:

$$[\Pi_p^{(m)}] \rightarrow [\Pi_{p+n/2}^{(m)}]$$

for $m$, the order of fixed momentum $\Pi$, divides $n$, the order of the full symmetry. The physical interpretation of these two operators will become apparent during the study of MBS at disclinations.

With the generalities out of the way, what follows in this section is a detailed construction of the rotation invariants for $C_4$ symmetric superconductors, as an explicit example, and a listing of the invariants for the remaining symmetries. The construction of the invariants for these other symmetries, however, can be found in detail in Ref [37].

**Fourfold Symmetry**

In fourfold symmetric systems there are two 2-fold fixed points $\Pi^{(2)} = X, X'$ and two 4-fold fixed points $\Pi^{(4)} = \Gamma, M$ in the Brillouin zone [see Fig. 3.2(a)]. However, the rotation spectra of $X$ and $X'$ are constrained to be the same by $C_4$ symmetry. Thus, we only need to take into account three sets of eigenvalues: $\Pi_1^{(4)} = e^{i\pi/4}, \Pi_2^{(4)} = e^{i3\pi/4}, \Pi_3^{(4)} = e^{-i3\pi/4}, \Pi_4^{(4)} = e^{-i\pi/4}$, for $\Pi^{(4)} = \Gamma, M$; and $X_1 = i, X_2 = -i$, as illustrated in Fig. 3.3.

![Figure 3.3: Rotation eigenvalues at the fixed-point momenta (a) $\Gamma$, (b) $X$, and (c) $M$ in the Brillouin zone of $C_4$ symmetric crystals.](image)

Following the form in Eq. 3.17 for the rotation invariants, we define them as follows:

$$[X_1] = #X_1 - (#\Gamma_1 + #\Gamma_3)$$

$$[X_2] = #X_2 - (#\Gamma_2 + #\Gamma_4)$$

$$[M_p] = #M_p - #\Gamma_p, \text{ for } p = 1, 2, 3, 4.$$
Now, we look at relations that reduce the number of required invariants, as follows:

(i) The total number of occupied states is constant over the Brillouin zone, which implies

\[ \sum_{p=1}^{2} \# X_p = \sum_{p=1}^{4} \# M_p = \sum_{p=1}^{4} \# \Gamma_p \]

or, in terms of the invariants defined above

\[ [X_1] + [X_2] = [M_1] + [M_2] + [M_3] + [M_4] = 0. \]

(ii) Since \( \hat{r}_n \) is a constant operator, its spectrum is the same at any of the rotation fixed points in the Brillouin zone. Therefore, since any state can be built from trivial bands with band inversions, the total number of states over both unoccupied and occupied bands having a particular rotation eigenvalue is the same at any of its fixed points. Since we have a total of 4 eigenvalues for \( \hat{r}_4 \) and 2 eigenvalues for \( \hat{r}_2 \), this relation can be captured in six equations, four equating the number of states with the same eigenvalue at the 4-fold fixed points \( \Gamma \) and \( M \), and two equating the number of states with the same eigenvalue at the 2-fold fixed points \( \Gamma \) and \( X \). However, PH symmetry reduces the number of necessary equations to three, because the PH operator sends a state in an occupied band and with rotation eigenvalue \( \Pi^{(n)}_p \) to an unoccupied band while changing its rotation eigenvalue to its complex conjugate \( \Pi^{(n)*}_p \). Thus, for example, \( \#M_1 \), which counts the number of occupied states with eigenvalue \( e^{i\pi/4} \), also counts the number of unoccupied states with eigenvalue \( e^{-i\pi/4} \) (see Fig. 3.4). The three equations are then

\[
\begin{align*}
\# M_1 + \# M_4 &= \# \Gamma_1 + \# \Gamma_4 \\
\# M_2 + \# M_3 &= \# \Gamma_2 + \# \Gamma_3 \\
\# X_1 + \# X_2 &= \# \Gamma_1 + \# \Gamma_2 + \# \Gamma_3 + \# \Gamma_4.
\end{align*}
\]

In the left hand side of the first equation, \( \# M_1 \) counts the number of states with eigenvalue \( e^{i\pi/4} \) in the occupied states at fixed point \( M \), while \( \# M_4 \) counts the number of states with eigenvalue \( e^{i\pi/4} \) in the unoccupied states at the fixed point \( M \) (see Fig. 3.4). Thus, the left hand side counts the total number of \( e^{i\pi/4} \) eigenvalues in the rotation operator at point \( M \). The right hand side counts the number of states having the same eigenvalue, but at the fixed point \( \Gamma \). Notice that the counting of states having eigenvalue \( e^{-i\pi/4} \) is given by the same expression. Similarly, the second equation counts the number
of states with eigenvalue $e^{i3\pi/4}$ (or with eigenvalue $e^{-i3\pi/4}$). The third relation equates the number of states with eigenvalue $i$ (or $-i$) at points $X$ and $\Gamma$. In terms of the invariants, the above relations reduce to

$[X_1] + [X_2] = [M_1] + [M_4] = [M_2] + [M_3] = 0$

of which Eq. 3.18 is a generalization. An illustration of the connection between unoccupied and occupied rotation eigenvalues is shown in Fig. 3.4.

Therefore, out of the six invariants defined initially, we are free to choose three which, along with the Chern number, identify the different topological classes of $C_4$ symmetric Hamiltonians:

$[X] = #X_1 - (#\Gamma_1 + #\Gamma_3)$

$[M_1] = #M_1 - #\Gamma_1$

$[M_2] = #M_2 - #\Gamma_2$  (3.22)

where the unnecessary subscript in $[X]$ has been omitted. We will see in Section 3.2.2 why we have not included the vector weak invariant as an independent invariant.

**Twofold Symmetry**

While in the case of fourfold symmetric superconductors two invariants are associated with the 4-fold fixed point $M$, in twofold symmetric systems only one is necessary because the number of complex conjugate pairs of eigenvalues of $\hat{r}_2$ at $M$ is half of those at $\hat{r}_4$ at $M$; however, in twofold symmetric systems we need to differentiate between eigenvalues at the 2-fold fixed points $X$ and $Y$, because they are not related as $X, X'$ for the fourfold symmetric case [see Fig. 3.2(a,b)]. Thus, in two-fold symmetric superconductors, three
rotation invariants are also necessary

\[
\begin{align*}
[X] &= \#X_1 - \#\Gamma_1 \\
[Y] &= \#Y_1 - \#\Gamma_1 \\
[M] &= \#M_1 - \#\Gamma_1.
\end{align*}
\] (3.23)

**Sixfold Symmetry**

In sixfold symmetric systems, 3-fold symmetry relates the 2-fold fixed points \(M, M',\) and \(M''\), while 2-fold symmetry relates the 3-fold fixed points \(K\) and \(K'\) [see Fig. 3.2(c)]. Imposing these constraints, the PH symmetry constraint, and demanding a constant number of bands across the Brillouin zone, we find that only two rotation invariants are required to classify \(C_6\) symmetric superconductors, defined as

\[
\begin{align*}
[M] &= \#M_1 - \#\Gamma_1 - \#\Gamma_3 - \#\Gamma_5 \\
\end{align*}
\] (3.24)

**Threefold Symmetry**

In 3-fold symmetric superconductors, the 2-fold fixed points \(M, M',\) and \(M''\) of 6-fold symmetric superconductors do not exist. Additionally, the 3-fold fixed points \(K\) and \(K'\) are not related by twofold symmetry [see Fig. 3.2(d)], and need to be differentiated by respective invariants, defined as

\[
\begin{align*}
[K] &= \#K_1 - \#\Gamma_1 \\
[K'] &= \#K'_1 - \#\Gamma_1.
\end{align*}
\] (3.25)

**Relation between invariants**

Any 4-fold symmetric system is also 2-fold symmetric and its \(C_2\) invariants are related to its \(C_4\) invariants by

\[
\begin{align*}
[M]^{(2)} &= [M_1^{(4)}] - [M_2^{(4)}] \\
[X]^{(2)} &= [Y]^{(2)} = [X]^{(4)}.
\end{align*}
\] (3.26)
Likewise, 6-fold symmetric superconductors have $C_3$ invariants, which are related to its $C_6$ invariants by

$$[K]^{(3)} = [K']^{(3)} = [K]^{(6)}.$$  (3.28)

### 3.2.2 Constraints on the Chern and weak invariants due to rotation symmetry

Rotation symmetry imposes constraints on the Chern and weak invariants. In superconductors with non-zero Chern invariant, the gauge transformation that relates the states in two neighboring rotational domains in the Brillouin zone is related to the rotation operator projected into the occupied bands at the fixed points $\Pi^{(n)}$. This allows us to determine the Chern number of an $n$-fold symmetric superconductor in terms of the rotation invariants mod $n$ as was done for 2D insulators in Refs. [18, 19, 34, 35]. These relations are

- $$Ch + 2[X] + [M_1] + 3[M_2] = 0 \mod 4$$  (3.29)
- $$Ch + [X] + [Y] + [M] = 0 \mod 2$$  (3.30)
- $$Ch + 2[K] + 3[M] = 0 \mod 6$$  (3.31)
- $$Ch + [K] + [K'] = 0 \mod 3$$  (3.32)

for $C_{4,2,6,3}$ symmetric superconductors respectively.

Regarding the weak $Z_2$ invariants in Eq. 3.10, rotation symmetry demands that the reciprocal lattice vector in Eq. 3.11 remain the same under rotation $G_\nu = R_\nu G_\nu$ (up to a reciprocal lattice vector). In $C_4$-symmetric systems we have $G_\nu = R_4 G_\nu$, which imposes the constraint that $\nu_1 = \nu_2 \equiv \nu$, since $\nu_1$, $\nu_2$ are defined mod 2. Thus, the index is

$$G_\nu = 2\pi \nu (b_1 + b_2) \left\{ \begin{array}{l} \nu = [X] + [M_1] + [M_2] \mod 2 \\ C_4 \text{ symm.} \end{array} \right.$$  (3.33)

In $C_2$-symmetric systems we have $G_\nu = R_2 G_\nu = -G_\nu$, which is compatible with $\nu_1$ and $\nu_2$ being defined modulo 2. The index is

$$G_\nu = 2\pi (\nu_1 b_1 + \nu_2 b_2) \left\{ \begin{array}{l} \nu_1 = [X] + [M] \mod 2 \\ \nu_2 = [Y] + [M] \mod 2 \\ C_2 \text{ symm.} \end{array} \right.$$  (3.34)

Finally, for $C_6$ and $C_3$ symmetric systems, the symmetry requirement is not compatible with the definition...
of the indices modulo 2. Thus, we have

$$G_\nu = 0 \bigg\{ C_6, C_3 \text{ symm.} \bigg\} \quad (3.35)$$

From these expressions it follows that the weak index is redundant in the topological classification, since it can be completely determined from the rotation invariants. The complete set of topological invariants consists of the Chern number, which must satisfy the rotational constraints above, and the set of rotation invariants for the particular rotation symmetry chosen.

### 3.3 Algebraic classification of topological crystalline superconductors

In this section, we first prove that the Chern invariant and rotation invariants completely stably classify 2D TCSs. It is necessary and sufficient that these quantities are identical in order for two rotation symmetric BdG Hamiltonians to be topologically equivalent. Furthermore, we discuss the free abelian additive structure of the topological classification of TCS and show that as a result all TCS can be topologically interpreted as certain combinations of simple decoupled models, which we call primitive generators. These model generators can be chosen to be simple Majorana lattice models or chiral $p$-wave SC’s. We construct primitive generators explicitly for $C_{2,3,4,6}$-symmetric superconductors in separate subsections.

#### 3.3.1 Complete Stable Classification of TCS and Algebraic Structure

Let us group the stable topological invariants for an $n$-fold rotation symmetric system into a vector form

$$\chi^{(n)}[H] = (Ch, \rho^{(n)}) \quad (3.36)$$

which lives in the (free abelian) $K$-group. Here we have denoted the rotation invariants of an $n$-fold symmetric system with an integer-valued vector $\rho^{(n)}$; specifically, $\rho^{(4)} = ([X],[M_1],[M_2])$; $\rho^{(2)} = ([X],[Y],[M])$; $\rho^{(6)} = ([M],[K])$; and $\rho^{(3)} = ([K],[K'])$, as shown in Sec. 3.2.1. $Ch$ is the Chern invariant in Eq. 3.9 that characterizes, for example, the edge chirality and thermal conductivity. The topological classification $\chi^{(n)}[H]$ implicitly depends on the pre-assigned PH and rotation operator $\Xi$ and $\hat{r}_n$. They are suppressed in the notation and abbreviated into the notation for the Hamiltonian $H = (H, \Xi, \hat{r}_n)$.

Two $n$-fold superconducting systems are stably equivalent if and only if they have the same topological...
invariants $\chi^{(n)}$. It is clear that two systems with distinct $\chi^{(n)}$’s must be stably inequivalent. This is because $\chi^{(n)}$ is unchanged under any continuous deformation that preserves the energy gap and symmetries as well as the addition of any trivial atomic bands. The converse of the statement can be proven by showing two systems with identical $\chi^{(n)}$ can be adiabatically connected up to trivial bands. There we show that there is no obstruction to adiabatically connecting two Hamiltonians with identical $\chi^{(n)}$.

3.3.2 Algebraic structure of TCS classification and primitive model generators

Given two $n$-fold symmetric superconductors with Hamiltonians $H_1$, $H_2$, rotation representations $\hat{r}_1$, $\hat{r}_2$, and PH operators $\Xi_1$, $\Xi_2$, which have topological invariants $\chi_1^{(n)}$ and $\chi_2^{(n)}$ respectively, their sum forms a third Hamiltonian $H_3 = H_1 \oplus H_2$, which preserves $n$-fold symmetry, represented by $\hat{r}_3 = \hat{r}_1 \oplus \hat{r}_2$, and has PH operator $\Xi_3 = \Xi_1 \oplus \Xi_2$. The form of the operators $\hat{r}_3$ and $\Xi_3$ implies that $H_3$ has the same labels $\Pi_p^{(n)}$ of its occupied states when compared to those of its constituent Hamiltonians $H_1$ and $H_2$; consequently, its rotation invariants are simply the addition of those for $H_1$ and $H_2$. Under this composition the Chern invariants simply add as well. Thus, the invariants for $H_3$ are given by

$$\chi^{(n)}[H_1 \oplus H_2] = \chi^{(n)}[H_1] + \chi^{(n)}[H_2].$$  \hspace{1cm} (3.37)

We see that a free abelian additive structure is associated with the topological classification, with elements given by the vectors in Eq. 3.36 and where the addition rule is given by Eq. 3.37. In mathematical terms, the association of $\chi^{(n)}$ to a Hamiltonian is an isomorphism between the $K$-group of stably equivalent classes of Hamiltonians and the free abelian group $\mathbb{Z}^N$ where the invariants $(Ch, \rho^{(n)})$ live. From this association, it follows that a set of primitive systems can be chosen which are capable of generating any TCS system up to stable equivalence. The only requirement for such a set of primitive generators $\{H_i^{(n)}\}$ is that their corresponding topological invariant vectors $\{\chi^{(n)}[H_i^{(n)}]\}$ form a basis for the free abelian group $(Ch, \rho^{(n)}) \in \mathbb{Z}^N$ associated with the topological classification of TCS with $n$-fold rotation symmetry. Once a set of primitive generators has been constructed, any system with Hamiltonian $H$ and invariant $\chi^{(n)}[H]$ can be made topologically equivalent to a unique combination of these generators

$$H \sim \bigoplus_{i} \left[ \bigoplus_{j=1}^{[\alpha_i]} \text{sgn}(\alpha_i)H_i^{(n)} \right].$$  \hspace{1cm} (3.38)
where $\{\alpha_i\}$ are the unique coefficients required by

$$
\chi^{(n)}[H] = \sum_i \alpha_i \chi^{(n)}[H_i^{(n)}] 
$$

(3.39)

and where similar compositions as the one for the Hamiltonian occur for the rotation representations and PH operators.

From this analysis, it follows that the topological characterization of any $C_n$ symmetric crystalline superconductor can be directly inferred from the characterization of any set of primitive generators. In what follows we present explicit primitive generators for each rotation symmetry.

### 3.3.3 Fourfold Symmetry

The classification of $C_4$ symmetric superconductors is given by

$$
\chi^{(4)} = (Ch, [X], [M_1], [M_2])
$$

(3.40)

subject to the constraint in Eq. 3.29. Since the rotation invariants determine the weak invariant, there are only 4 linearly independent indices that span all possible topological classes. Thus, we need 4 primitive generators.

The first two generators correspond to two topologically distinct phases of a spinless, chiral $p_x + ip_y$ superconductor on a square lattice with 1st and 2nd nearest-neighbor hopping terms

$$
H_{u_1, u_2}^{(4)}(\mathbf{k}) = \Delta \left[ \sin (\mathbf{k} \cdot \mathbf{a}_1) \tau_x + \sin (\mathbf{k} \cdot \mathbf{a}_2) \tau_y \right] 
+ u_1 \left[ \cos (\mathbf{k} \cdot \mathbf{a}_1) + \cos (\mathbf{k} \cdot \mathbf{a}_2) \right] \tau_z 
+ u_2 \left[ \cos (\mathbf{k} \cdot \mathbf{a}_1') + \cos (\mathbf{k} \cdot \mathbf{a}_2') \right] \tau_z
$$

(3.41)

where $\tau_x$, $\tau_y$, and $\tau_z$ are Pauli matrices that act on the Nambu degree of freedom, $\mathbf{a}_1 = a(1,0)$ and $\mathbf{a}_2 = a(0,1)$ are primitive vectors for the square lattice, and $\mathbf{a}_1' = \mathbf{a}_1 + \mathbf{a}_2$, $\mathbf{a}_2' = -\mathbf{a}_1 + \mathbf{a}_2$ are orthogonal vectors connecting second-nearest-neighbor sites. $\Delta$ is the $p_x + ip_y$ pairing and $u_1$ and $u_2$ are nearest and second-nearest neighbor hopping amplitudes respectively. The pairing and nearest-neighbor hopping terms give a gapless Hamiltonian with Dirac cones at the 2-fold fixed points $X$ and $X'$. To open the gap, second-nearest-neighbor hopping terms are also considered. The gap closing for $u_2 = 0$ causes a phase transition and another phase transition exists at $u_1 = u_2$, where a Dirac cone appears at the 4-fold fixed point $M$. Finally, a third transition occurs at $u_1 = -u_2$, where a Dirac cone appears at the 4-fold symmetric point $\Gamma$. Fig. 3.5 shows the phases of the
Figure 3.5: Topological phases of model $H_{u_1,u_2}^{(4)}$ in Eq. 3.41. At $u_2 = u_1$ the gap closes at the 4-fold fixed point $M$, at $u_2 = -u_1$, the gap closes at $\Gamma$. At $u_2 = 0$ the gap closes at $X$ and $X'$. Chern numbers and weak invariants are shown for each phase. For rotation invariants, see Table 3.1. Primitive generators $H_1(4)$ and $H_2(4)$ we simulated with parameters as shown by the cross and asterix respectively.

model, and the corresponding Chern invariants and weak indices.

We take the first two primitive models to have Hamiltonians

$$H_1^{(4)} = H_{u_1,u_2}^{(4)} \text{ for } u_1 > u_2 > 0$$
$$H_2^{(4)} = H_{u_1,u_2}^{(4)} \text{ for } -u_1 > u_2 > 0$$

and PH and rotation operators given by

$$\Xi_{1,2} = \tau_x K, \quad \hat{r}_{1,2} = \pm e^{i\pi \tau_z}$$

where $K$ is complex conjugation. The rotation operator obeys $\hat{r}_{1,2}^\dagger H(R_4 k) \hat{r}_{1,2} = H(k)$ where

$$R_4 = \begin{pmatrix} \cos(\pi/2) & \sin(\pi/2) \\ -\sin(\pi/2) & \cos(\pi/2) \end{pmatrix} = e^{i\pi \sigma_y}$$

is the 4-fold rotation matrix acting on $k$ space. These two generators break time reversal symmetry (TRS). Both have $Ch = 1$, and exhibit edge modes in a strip geometry as shown in Fig. 3.6. $H_1^{(4)}$ has $G_\nu = 0$, while $H_2^{(4)}$ has $G_\nu = b_1 + b_2$. The rotation invariants for these two generators are shown in Table 3.1.

The other two primitive generators are 2D generalizations of Kitaev’s p-wave wire [93] with 4 Majorana
Figure 3.6: Energy bands for primitive Hamiltonians (a) $H^{(4)}_1$ and (b) $H^{(4)}_2$ for a strip geometry with periodic boundary conditions in the $a_1$ direction and open boundary conditions in the $a_2$ direction. The dashed blue/ dotted red lines correspond to states localized at the upper/lower edges. The parameters are $u_1/\Delta = 1, u_2/\Delta = 0.5$ for (a), and $u_1/\Delta = -1, u_2/\Delta = 0.5$ for (b). Both models have $Ch = 1$.

fermions per site

\[ H^{(4)}_3 = i\Delta \sum_r \left( \gamma^1_{r+r+a_1} \gamma^3_{r+r+a_1} + \gamma^2_{r-r+a_2} \gamma^4_{r-r+a_2} \right) \]
\[ H^{(4)}_4 = i\Delta \sum_r \left( \gamma^1_{r+r+a'_1} \gamma^3_{r-r+a'_1} + \gamma^2_{r-r+a'_2} \gamma^4_{r+r+a'_2} \right) \] (3.44)

where the $\gamma^i_r$'s are Majorana operators at site $r$, for $i = 1, 2, 3, 4$. These operators obey $\gamma^i_r \gamma^j_{r'} = \delta_{ij} \delta_{r_1,r_2}$. Figs. 3.7(a,b) depict these two models.

The rotation operator for these two models is

\[ \hat{r}_{3,4} = \prod_r e^{-\frac{\pi}{2} \gamma^1_{r-r'} \gamma^2_{r-r'} e^{-\frac{\pi}{2} \gamma^3_{r-r'} \gamma^4_{r-r'}}} \] (3.45)

which transforms the Majorana operators as $\hat{r}_{3,4} \left( \gamma^1_{r-r'}, \gamma^2_{r-r'}, \gamma^3_{r-r'}, \gamma^4_{r-r'} \right) \hat{r}^\dagger_{3,4} = \left( \gamma^2_{Rr}, \gamma^3_{Rr}, \gamma^4_{Rr}, -\gamma^1_{Rr} \right)$. If we change the basis into complex fermionic operators at each site $c = (\gamma^1 + i\gamma^3)/2$, and $d = (\gamma^2 + i\gamma^4)/2$, the Hamiltonians in momentum space are

\[ H^{(4)}_3(k) = \Delta (\cos(k \cdot a_1) \tau_z + \sin(k \cdot a_1) \tau_y) \oplus \Delta (\cos(k \cdot a_2) \tau_z + \sin(k \cdot a_2) \tau_y) \]
\[ H^{(4)}_4(k) = \Delta (\cos(k \cdot a'_1) \tau_z + \sin(k \cdot a'_1) \tau_y) \oplus \Delta (\cos(k \cdot a'_2) \tau_z + \sin(k \cdot a'_2) \tau_y) \] (3.46)

where the basis $\xi_k = \left( c_k, c^\dagger_{-k}, d_k, d^\dagger_{-k} \right)^T$ has been used. The PH and rotation operators in this basis are

\[ \Xi_{3,4} = \begin{pmatrix} \tau_x & 0 \\ 0 & \tau_x \end{pmatrix}, \quad \hat{r}_{3,4} = \begin{pmatrix} 0 & -i\tau_z \\ i\tau_z & 0 \end{pmatrix} \] (3.47)
Figure 3.7: Tight binding representations of primitive generators that take the form of 2D p-wave wires for various rotation symmetries. (a) $H_3^{(4)}$, (b) $H_4^{(4)}$, (c) $H_4^{(2)}$, and (d) $H_6^{(6)}$. Black dots indicate Majorana fermions. $H_3^{(4)}$ and $H_4^{(4)}$ are 4-fold symmetric superconductors with 4 Majorana fermions per site and 1st and 2nd nearest-neighbor connections respectively. $H_4^{(2)}$ has the same atomic arrangement as in (a,b), but contains only two Majorana fermions per site and is trivial along $a_2 = (0,1)$. Gray vertical lines in (c) serve only as a guide and do not represent terms in the Hamiltonian. $H_6^{(6)}$ is a 6-fold symmetric superconductor with 6 Majorana fermions per site.

where $\tau_0$ is the $2 \times 2$ identity matrix acting on the Nambu degree of freedom.

### 3.3.4 Twofold Symmetry

The classification of $C_2$ symmetric superconductors is given by

$$\chi^{(2)} = (Ch, [X], [Y], [M])$$

subject to the constraint in Eq. 3.30. For simplicity, we take three of the $C_4$ symmetric models described above as our first three $C_2$ generators

$$H_1^{(2)} = H_1^{(4)}$$
$$H_2^{(2)} = H_2^{(4)}$$
$$H_3^{(2)} = H_3^{(4)}.$$  \hfill(3.49)

Generator $H_4^{(4)}$ is in the same class as $H_3^{(4)}$ when $C_4$ symmetry is forgotten. Since these three first generators are $C_4$ symmetric, they have $[X] = [Y]$, thus, the fourth generator must break $C_4$ symmetry. We take it to be a 2-dimensional anisotropic array of p-wave wires

$$H_4^{(2)} = i\Delta \sum_{r} \gamma_r^{1} \gamma_r^{2} a_z$$  \hfill(3.50)
where \( \mathbf{r} \) runs over all lattice sites spanned by the primitive vectors \( \mathbf{a}_1 = a(1,0), \mathbf{a}_2 = a(0,1) \). This model is trivial along \( \mathbf{a}_2 \), and is depicted in Fig. 3.7(c). Its rotation operator is

\[
\hat{r}_4 = \prod_{\mathbf{r}} e^{-\frac{\pi}{2} \gamma_1 r_x \gamma_2 r_x} \tag{3.51}
\]

which transforms the Majorana operators as \( \hat{r}_4 (\gamma_1 r_x, \gamma_2) \hat{r}_4^\dagger = (\gamma_2 r_x, -\gamma_1 r_x) \). In terms of the complex fermion operators \( c = (\gamma_1 + i \gamma_2)/2 \), the generator \( H_4^{(2)} \) in momentum space is

\[
H_4^{(2)}(\mathbf{k}) = \Delta (\cos (\mathbf{k} \cdot \mathbf{a}_1) \tau_z + \sin (\mathbf{k} \cdot \mathbf{a}_1) \tau_y) \tag{3.52}
\]

in the basis \( \xi_{\mathbf{k}} = (c_{\mathbf{k}}, c_{-\mathbf{k}}^\dagger) \map{T} \). The PH and rotation operators become

\[
\Xi_2 = \tau_z K, \quad \hat{r}_4 = -i \tau_z. \tag{3.53}
\]

The invariants for all the \( C_2 \) primitive generators are shown in Table 3.1.
Figure 3.8: Topological phases of model \( H^{(6)} \) in Eq. 3.55. For rotation invariants see Table 3.1. Primitive generators \( H_1^{(6)} \) and \( H_2^{(6)} \) were simulated with parameters marked by the cross and asterix respectively.

### 3.3.5 Sixfold Symmetry

The topology of \( C_6 \) symmetric superconductors is characterized by

\[
\chi^{(6)} = (Ch, [M], [K]).
\]

subject to the constraint in Eq. 3.31. The first two models are spinless, chiral \( p_x + i p_y \) superconductors on a hexagonal lattice with 1st and 2nd nearest-neighbor hopping terms. The generic Hamiltonian from which these two models are taken is

\[
H_{u_1,u_2}^{(6)}(k) = \sum_{i=1}^{3} \left[ \Delta \sin (k \cdot a_i) a_i \cdot \tau + u_1 \cos (k \cdot a_i) \tau_z + u_2 \cos (k \cdot a'_i) \tau_z \right]
\]

where \( \tau = (\tau_x, \tau_y) \) acts on Nambu space; \( a_1 = a(1,0) \), \( a_2 = a (-1/2, \sqrt{3}/2) \), \( a_3 = -(a_1 + a_2) = a (-1/2, -\sqrt{3}/2) \) are primitive lattice vectors of a triangular lattice; and \( a'_1 = a_2 - a_1 \), \( a'_2 = a_3 - a_2 \), \( a'_3 = a_1 - a_3 \) are vectors connecting second-nearest-neighbor sites in the lattice. \( \Delta \) is the \( p_x + i p_y \) pairing, and \( u_1, u_2 \) are nearest and second-nearest neighbor hopping amplitudes. The Hamiltonian is gapped for nonzero \( u_1 \) or \( u_2 \), except at \( u_1 = -u_2 \), where there is a phase transition with Dirac cones appearing at the 6-fold and 2-fold symmetric points \( \Gamma \) and \( M \), and at \( u_1 = 2u_2 \), where another transition occurs, in which a Dirac cone appears at the 3-fold symmetric point \( K \). Fig. 3.8 shows the phases of the model with its Chern invariants. The weak index \( G_\nu \) for any \( C_6 \) symmetric superconductor is zero.
Figure 3.9: Energy bands for primitive Hamiltonians (a) $H_{1}^{(6)}$ and (b) $H_{2}^{(6)}$ for a strip geometry with periodic boundary conditions in the $a_1$ direction and open boundary conditions in the $(0,1)$ direction. The dashed blue/ dotted red lines correspond to states localized at the upper/lower edges. The parameters are $u_1/\Delta = 1$, $u_2 = 0$ for (a) and $u_1 = 0$, $u_2/\Delta = 1$ for (b). The Chern invariants are 1 and 3 respectively.

We take the first two primitive models to be

$$H_{1}^{(6)} = H_{u_1,u_2}^{(6)} \quad \text{for} \quad \frac{1}{2}u_2 > u_1 > -u_2, \ u_1 > 0$$

$$H_{2}^{(6)} = H_{u_1,u_2}^{(6)} \quad \text{for} \quad \begin{cases} u_2 > \frac{1}{2}u_1 & \text{if} \ u_1 > 0 \\ u_2 > -u_1 & \text{if} \ u_1 < 0 \end{cases}$$

which belong to different topological classes, as shown by their invariants in Table 3.1. $H_{1}^{(6)}$ and $H_{2}^{(6)}$ have Chern invariants 1 and 3 respectively, with edge modes in a strip geometry as shown in Fig. 3.9. The PH and rotation operators are

$$\Xi_{1,2} = \tau_zK, \quad \hat{r}_{1,2} = e^{i\frac{\pi}{6}\tau_z}$$

so that $\hat{r}_{1,2}^\dagger H(R_6\mathbf{k})\hat{r}_{1,2} = H(\mathbf{k})$ where $R_6 = \exp(i\frac{\pi}{3}\sigma_y)$ is the 6-fold rotation matrix.

The third model is a 2D generalization of Kitaev’s p-wave wire

$$H_{3}^{(6)} = i\Delta \sum_r \left( \gamma_1^r \gamma_4^r + \gamma_2^r \gamma_5^r + \gamma_3^r \gamma_6^r \right)$$

with rotation operator

$$\hat{r}_3 = \prod_r e^{-\frac{\pi}{2} \gamma_1^r \gamma_8^r e^{-\frac{\pi}{2} \gamma_5^r \gamma_8^r e^{-\frac{\pi}{2} \gamma_3^r \gamma_8^r e^{-\frac{\pi}{2} \gamma_2^r \gamma_8^r e^{-\frac{\pi}{2} \gamma_4^r \gamma_8^r e^{-\frac{\pi}{2} \gamma_6^r \gamma_8^r}}}}}$$

that transforms the Majorana fermions as $\hat{r}_3^\dagger \gamma_i^r \hat{r}_3 = \gamma_i^r$ for $i = 1, 2, 3, 4, 5$ and $\hat{r}_3^\dagger \gamma_6^r \hat{r}_3 = -\gamma_6^r$. Fig. 3.7(d) depicts an illustration of this model. In terms of the complex fermion operators $c = (\gamma^3 + i\gamma^4)/2$, $d =
\[(\gamma^2 + i\gamma^5)/2, \ \epsilon = (\gamma^3 + i\gamma^6)/2\] the Hamiltonian in momentum space is

\[H_3^{(6)}(k) = \sum_{i=1}^{3} \Delta(\cos(k \cdot a_i) \tau_z + \sin(k \cdot a_i) \tau_y)\]  

written in the basis \(\xi_k = (c_k, c_{-k}^\dagger, d_k, d_{-k}^\dagger, e_k, e_{-k}^\dagger)^T\). The PH and rotation operators in this basis are

\[\Xi_3 = \begin{pmatrix} \tau_x & 0 & 0 \\ 0 & \tau_x & 0 \\ 0 & 0 & \tau_x \end{pmatrix}, \quad \tilde{r}_3 = \begin{pmatrix} 0 & 0 & -i\tau_z \\ 0 & \tau_0 & 0 \\ 0 & 0 & \tau_0 \end{pmatrix}.\]

Its invariants are shown in Table 3.1.

### 3.3.6 Threefold Symmetry

\(C_3\)-symmetric superconductors are classified by

\[\chi^{(3)} = (Ch, [K], [K'])\]

subject to the constraint in Eq. 3.32. Thus, we need three primitive models. Just as we inherit \(C_4\) primitive generators as generators for the \(C_2\) symmetry, we take advantage of the \(C_3\)-symmetry present in any \(C_6\) crystal and take the first two generators to be the first two generators of the \(C_6\) classification

\[H_1^{(3)} = H_1^{(6)}, \quad H_2^{(3)} = H_2^{(6)}\]

with PH and rotation operators

\[\Xi_{1,2} = \tau_z K, \quad \tilde{r}_{1,2} = e^{i\pi\tau_z}.\]

Because these two generators are \(C_6\) symmetric, they have \([K] = [K']\). The third generator will need to break \(C_6\) symmetry, so that \([K] \neq [K']\). This third generator is a spinless, chiral, \(p_x + ip_y\) superconductor with 1st nearest-neighbor hopping and pairing terms

\[H_3^{(3)}(k) = \sum_{i=1}^{3} [\Delta \sin(k \cdot a_i) a_i \cdot \tau + u_1 \sin(k \cdot a_i) \tau_z] + \mu \tau_z, \quad \text{for} \ 0 < \mu < \frac{\sqrt{3}}{2} u_1\]

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Figure 3.10: Energy bands for primitive generator with Hamiltonian $H_3^{(3)}$ for a strip geometry with periodic boundary conditions in the $a_1$ direction and open boundary conditions in the (0,1) direction. The dashed blue/dotted red lines correspond to states localized at the upper/lower edges. The parameters are $u_1/\Delta = 0.5$, and $\mu/\Delta = 0.5$. This model has Chern invariant -1.

where $\Delta$ is the pairing amplitude, $u_1$ is the 1st nearest-neighbor hopping amplitude, and $\mu$ is the Fermi energy. $\mu$ is restricted to the indicated range to avoid closing gaps at the fixed point $\Gamma$ and at the three fixed points $M$ when $\mu = 0$, and additionally at the fixed point $K$ when $\mu = \sqrt{3}/2$. $H_3^{(3)}$ has the PH and rotation operators of Eq. 3.64.

The invariants for these three primitive models are shown in Table 3.1.

3.4 Disclination-dislocation fractional vortex composite

We now review the topological classification of point defects in a two-dimensional discrete lattice. Dislocations in a system with broken translation symmetry are torsional singularities characterized by Burgers’ vectors. Disclinations in a system with broken rotation symmetry are curvature singularities characterized by Frank angles. These quantities are discrete translation and rotation holonomies picked up by a particle going once around the point defect. [129, 130, 131, 132, 124, 133] In superconductors where $U(1)$ charge conservation symmetry is broken, isolated flux vortices are quantized in units of $q(hc/2e)$, for integer $q$, because the Berry phase accumulated by a quasi-particle going around a cycle must be real (it is $(-1)^q$ for these vortices). These holonomies are path independent, and therefore topological. In this section, we describe the classification of composite point defects in crystalline superconductors, which are mixtures of dislocations, disclinations, and fractional vortices. The “fractional” vortices we discuss below do not have to be quantized in units of $hc/2e$ because they appear as composite defects bound to disclinations.

The discrete rotation $\hat{r}_a$ and lattice translations $T_a$ by Bravais vector $a$ that generate the fermionic space
Figure 3.11: Lattice disclinations and dislocations. (a,b) Dislocations in the form of disclination dipoles. (c,d) ±120° disclinations with opposite Frank angles and different translation types.

Figure 3.12: Holonomy of a disclination around a loop (red path) with a fixed starting point (blue dot).

group $\tilde{P}n = \tilde{C}_n \ltimes \mathcal{L}$ obey the non-Abelian group relations

$$\tilde{P}n = \left\langle \hat{r}_n, T_a \right| \hat{r}_n^n = -1, T_a T_b = T_{a+b}, \hat{r}_n T_a \hat{r}_n^{-1} = T_{R_n a} \right\rangle \quad (3.66)$$

where $R_n = e^{2\pi i \sigma_y / n}$ is the rotation matrix on real space.

The holonomy of a closed path is the amount of translation and rotation accumulated by parallel transporting a frame around the loop. An example is given in Fig. 3.12 where the $xy$-frame is rotated by 90° at every corner. Its holonomy is given by $\hat{r}_4 T_{3e_x} \hat{r}_4 T_{3e_x} \hat{r}_4 T_{3e_x} = T_{-3e_x} \hat{r}_4^3$. In general, the holonomy of a closed path is an element $T_a \hat{r}(\Omega)$ in the space group $\tilde{P}n$, for $\hat{r}(\Omega) = \hat{r}_n^m$ and $\Omega = 2\pi m/n$ is the Frank
Holonomy is path independent as long as the starting and ending points of the path are fixed and the trajectory counter-clockwisely circles the defect once.

If we change the starting point of our closed path the holonomy is transformed according to conjugacy upon a translation $T_c$ of the fixed point.

$$T_{\alpha}(\Omega) \rightarrow T_c [T_{\alpha}(\Omega)] T_{-c} = T_{\alpha+(1-R(\Omega))} e^{\hat{r}(\Omega)} \quad (3.67)$$

where $R(\Omega)$ is the rotation matrix $e^{i\Omega \sigma_y}$. Since the topological classification of the defects should not depend on where we arbitrarily begin our path, point defects are thus topologically classified by conjugacy classes of holonomy denoted by $(\Omega, [a])$. The Frank angle $\Omega$ is the rotation piece that characterizes the curvature singularity of the conical disclination, this quantity is always independent of the starting point of the path. The translation piece, which is transformed when the starting point is moved, is reduced to the equivalence class $[a]$ which lies in the quotient:

$$\frac{\mathcal{L}}{(R(\Omega) - 1)\mathcal{L}} = \left\{ \begin{array}{ll}
\mathcal{L}, & \text{for } \Omega = 0 \\
0, & \text{for } \Omega = \pm 60^\circ \\
\mathbb{Z}_2, & \text{for } \Omega = \pm 90^\circ \\
\mathbb{Z}_3, & \text{for } \Omega = \pm 120^\circ \\
\mathbb{Z}_2 \oplus \mathbb{Z}_2, & \text{for } \Omega = 180^\circ 
\end{array} \right. \quad (3.68)$$

where we recall that $\mathcal{L}$ is the discrete translation group.

Analogous to the Burgers’ vector, $[a]$ is the translation piece of the holonomy that characterizes the torsional part of the singularities. This table implies that for dislocations, i.e., the case when $\Omega = 0$, the holonomy can lie in the full translation group and is not affected by moving the path starting point. For the other cases, which all have non-zero Frank angles, the quotient elements identify possible inequivalent rotation centers, e.g., a vertex or square plaquette in a fourfold lattice; a vertex, a rectangular plaquette, or the mid-point of a horizontal or vertical edge in a twofold lattice; a hexagonal plaquette or the two sublattice vertices of a threefold honeycomb lattice. Heuristically, this implies that the translational part of the holonomy of a disclination changes when the starting point of the path is chosen, but in all cases except for $\Omega = 60^\circ$, some piece of the translation remains invariant. For example, for the $C_4$ case with $\Omega = \pi/2$ the translation holonomy can be modified by choosing a different starting point, but the parity, i.e., the evenness or oddness of the total number of translations always remains fixed. Since the rotation symmetry is $C_4$ we do not distinguish between translations in the $x$ or $y$ direction and thus we only know the total parity of all
The set of equivalence classes is also distinguished by the properties at the core of the disclination, which must lie at a rotation center of the lattice. For lattices with multiple rotation centers, it provides a further topological distinction of disclinations with the same Frank angle (i.e. curvature). In fourfold-symmetric lattices, a $\mathbb{Z}_2$ translation piece is defined, which counts the evenness or oddness of the number of discrete translations picked up while circulating along the closed path. We can use this translation piece to provide type-labels for disclinations: we can label $\Omega = \pm \pi/2$ disclinations as type-(0,0) disclinations, for those having an even number of translations along both primitive axes of the crystal, or type-(1,0) disclinations, for those having an odd number of translations along the primitive axis $a_1$ and an even number of translations along $a_2$ (recall that in $C_4$ symmetric systems, type-(0,1) disclinations are equivalent to type-(1,0) disclinations, as they are related by an arbitrary choice of reference frame). Microscopically, type-(0,0) $\Omega = \pm \pi/2$ disclinations center at a vertex with odd coordination number while a type-(1,0) $\Omega = \pm \pi/2$ disclinations center at an odd-sided plaquette [see Fig. 3.11(a)]. On a more macroscopic level, we can see that there is a topological obstruction to coloring the lattice with a checkerboard plaquette pattern around a type-(0,0) $\Omega = \pm \pi/2$ disclination. In disclinations of twofold-symmetric lattices, the $\mathbb{Z}_2 \oplus \mathbb{Z}_2$ translation piece corresponds to type-(0,0), type-(1,0), type-(0,1), and type-(1,1) disclinations with Frank angle $\Omega = \pm \pi$, which count the evenness or oddness of translations along the $(x, y)$ direction of the crystal. For threefold-lattices, the $\mathbb{Z}_3$ translation piece counts the number of discrete translations modulo 3 along the closed path. An $\Omega = \pm \pi/3$ disclination in a honeycomb lattice can center at a square or octagon plaquette for type-0 [Fig. 3.11(c)] or one of the bipartite vertices for type-1 and 2 [Fig. 3.11(d)]. Type-1,2 $\Omega = \pm \pi/3$ disclinations are topological obstructions to plaquette tri-coloration.

In general, the Frank angle $\Omega$ is defined modulo $4\pi$ in a fermionic system. The holonomy around an $\Omega$-disclination differs from that of an $\Omega + 2\pi$ one by the Berry phase $-1$. In a crystalline superconductor, disclinations can bind quantum vortices as composite point defects. For example, the primitive model Hamiltonians discussed in this Chapter are $p$-wave and thus the rotation and superconducting orders are...
intertwined; all rotation operators $\hat{r}_n$ contain the factor $e^{i\pi \tau z/n}$ that involves the Nambu $\tau$-degree of freedom. As a result, an $\Omega$-disclination necessarily binds a fractional vortex with quantum number $q = \frac{\Omega}{2\pi}$ modulo $2\mathbb{Z}$. And therefore an $\Omega$-disclination differs from a $\Omega + 2\pi$ one by an (odd integer multiple of) $hc/2e$ vortex. Our result can thus be viewed as a gravitational generalization of Read and Green’s magnetic vortex MBS [95].

In order to derive our index theorem results below we must understand the details of combining defects into composite defects. Multiple point defects can be classically fused into a single composite defect that is holonomically characterized by a loop encircling all its constituents. The fusion between a pair of defects depends on their individual classification as well as the distance of separation. Suppose $T_{a_i} \hat{r}(\Omega_i)$ are the holonomies of defects $i = 1, 2$ calculated from starting points separated by the lattice vector $d$. The overall holonomy is given by

\[
(\Omega_1, a_1) \cdot (\Omega_2, a_2) = (\Omega_1 + \Omega_2, a_1 + R(\Omega_1)(a_2 + (R(\Omega_2) - 1)d)).
\] (3.69)

This cleanly reduces to the addition rule $a_1 + a_2$ for Burgers’ vectors of dislocations when $\Omega_1 = \Omega_2 = 0$.

As another example, the equation also shows that the Burgers’ vector characterizing a disclination dipole $\Omega_1 = -\Omega_2 = \Omega$ [see Fig. 3.11(a,b)] grows linearly in the separation $d$.

\[
B_{dipole} = a_1 + a_2 + [R(\Omega) - 1](a_1 - d).
\] (3.70)

However, for disclinations we have seen that the total translation holonomy depends on the starting point of the chosen path, and nicely, the equivalence class of the Burgers’ vector as an element in the quotient $L/R(\Omega)$ is independent from the last term so that $[B] = [a_1] + [a_2]$. For instance, as we will show below and have shown in Ref. [124], in a twofold or fourfold symmetric lattice the number of MBS at a disclination dipole is predicted by the index theorem

\[
\Theta_{dipole} = \frac{1}{2\pi} B \cdot G_\nu = \frac{1}{2\pi} (a_1 + a_2) \cdot G_\nu \mod 2
\] (3.71)

and is independent of the disclination separation $d$. As we have shown in Ref. [133], when $\Theta_{dipole}$ is non-zero, this result implies there must be an uneven distribution of MBS among the pair of disclinations, i.e., only one of them has an odd number of MBS and the other has an even number.
3.5 Majorana zero modes at disclinations

We will now use the existence (or non-existence) of MBS in the primitive generators, which were defined for each symmetry class in Sec. 3.3, to construct $\mathbb{Z}_2$ index theorems. These index theorems determine the parity of the number of Majorana bound states (MBS) trapped at disclinations. There is a separate index for each symmetry and the index $\Theta^{(n)}$ for a $C_n$ symmetric system is a function of the topological class of the system $\chi^{(n)}$ and the holonomy that characterizes the disclination $(\Omega, T)$.

To determine the index theorems we must use two essential results. The first is that under the combination of disclinations centered at the same point, the index obeys

$$\Theta (\chi, (\Omega_1, T_1) \circ (\Omega_2, T_2)) = \Theta (\chi, (\Omega_1 + \Omega_2, T_1 + R(\Omega_1)T_2)) \mod 2$$

(3.72)

which results from Eq. 3.69 with vanishing separation $d$ between disclinations. The second result is that the index is linear modulo 2 under the addition of $C_n$ symmetric systems, i.e., for two superconductors with Hamiltonians $H^{(n)}_1, H^{(n)}_2$ in classes $\chi^{(n)}_1, \chi^{(n)}_2$ respectively that are combined into a superconductor with Hamiltonian $H^{(n)}_1 \oplus H^{(n)}_2$ that belongs to the topological class $\chi^{(n)}_1 + \chi^{(n)}_2$, the index is

$$\Theta (\chi_1 + \chi_2, (\Omega, T)) = [\Theta (\chi_1, (\Omega, T)) + \Theta (\chi_2, (\Omega, T))] \mod 2.$$  

(3.73)

Thus, finding the parity of MBSs at disclinations for the primitive generators of $C_n$ symmetric superconductors naturally provides a characterization of the parity of MBSs at disclinations in any $C_n$ symmetric system. Our task then reduces to finding the parity of MBS for the primitive generators of Sec. 3.3.

Two different approaches were used to this end, depending on the type of model. For the spinless chiral $p_x + ip_y$ generators $H^{(4)}_1, H^{(4)}_2, H^{(6)}_1, H^{(6)}_2, H^{(3)}_1, H^{(3)}_2$ and $H^{(3)}_3$, we numerically simulated the systems. Since all of the generators break time-reversal symmetry we constructed lattice models without open boundaries, thus avoiding the presence of edge modes. The total curvature in such a compact surface $S$ without boundaries is given by the Gauss-Bonnet theorem

$$\int_S K dA = 2\pi(2 - 2g)$$

(3.74)

where $K$ is the Gaussian curvature of the surface and $g$ the surface’s genus. Since disclinations of Frank angle $\Omega$ induce a curvature $\Omega$ on the lattice, we found that toric configurations, which have $g = 1$ and thus no overall curvature, minimized the number of disclinations needed for all symmetries. Disclinations
with opposite Frank angles were used, both to flatten the total curvature and to ensure that the total superconducting flux is zero over the unit cells.

For the generators that take the form of 2D p-wave wire models, e.g., $H_3^{(4)}$, $H_4^{(4)}$, $H_4^{(2)}$, and $H_3^{(6)}$, no simulations were used. Instead, we take advantage of the fact that the parity of the number of MBS at a defect is insensitive to perturbations that preserve the gap and the rotation symmetry away from the defect. This is true because if these conditions are satisfied it implies that there are no low-energy channels that would allow a single MBS to escape the defect core. Thus, we can determine the parity of MBSs “pictorially” in a simple tight-binding limit. In what follows, we describe our findings for each symmetry separately.

### 3.5.1 Fourfold symmetry

Two hexagonal lattice cells were chosen for the simulation of $H_1^{(4)}$ and $H_2^{(4)}$, as shown in Fig. 3.14(a,b). The first lattice cell contains only $\Omega = -\pi/2$ type-(1,0) and $\Omega = +\pi$ type-(1,1) disclinations, as in Figs. 3.14(c,d) [we say type-(1,1) instead of (0,0) because we will also use this lattice to discuss the $C_2$ invariant classification, for $C_4$ they are the same]. In the second lattice cell the disclination of type-(1,0) at point $O_1$ is replaced by one of type-(0,0), and the disclination of type-(1,1) at point $K$ is replaced by one of type-(1,0), while the disclination type at point $O_2$ is maintained. The disclinations for the second lattice cell look as in Figs. 3.14(c,e,f). Notice that in both cases one $\Omega = +\pi$ and two $\Omega = -\pi/2$ disclinations exist per unit cell, which amount to no global curvature, thus allowing us to impose periodic boundary conditions by identifying the opposite sides of the hexagon, in a flat-curvature toric structure.

The parameters used in the simulations were $2u_2/\Delta = \pm u_1/\Delta = 1$ for $H_1^{(4)}$ and $H_2^{(4)}$ respectively. We did not find unpaired MBSs for the case of $H_1^{(4)}$, and found unpaired MBSs only for type-(1,0) disclinations with Frank angles $\Omega = -\pi/2$ and $\pi$ in the case of $H_2^{(4)}$. Fig. 3.15 shows the density of states and probability density functions for the zero-modes in the simulation of $H_2^{(4)}$ for the configuration in Fig. 3.14(a).

In order to derive the topological index for $C_4$ symmetric superconductors, we consider $\Omega = -\pi/2$ disclinations only, and use the results at $\Omega = \pi$ disclinations for the derivation of the index for $C_2$ symmetric superconductors later on (recall that the first three generators for the $C_4$ and $C_2$ classifications are the same). The parity of MBS in the 2D p-wave wire models $H_3^{(4)}$ and $H_4^{(4)}$ at both types of $\Omega = -\pi/2$ disclinations can be found pictorially, as shown in Fig. 3.16. Majorana fermions are represented by black dots, unless they are unpaired, in which case they are red open circles. $H_3^{(4)}$ has unpaired MBS for type-(0,0) disclinations, and $H_3^{(4)}$ has them for both types. Notice that in the cases where odd Majorana fermions are found at the core, there is also an odd number of Majorana fermions at the boundary. The findings for all $C_4$ primitive models are summarized in Table 3.2.
Figure 3.14: (a,b) Unit cells of $C_4$-symmetric lattice configurations having $-\pi/2$ and $+\pi$ disclinations. Periodic boundary conditions are imposed, by identifying edges on the unit cell with red, blue and black lines. (c-f) Flattened cores of $\Omega = -\pi/2$ (c,e) and $\Omega = +\pi$ (d,f) disclinations centered at points $O, K, O'$, and $K'$ in the unit cells. The disclination types are: type-(1,0) in (c) and (f), type-(1,1) in (d), and type-(0,0) in (e).

From these results, and appealing to the linearity of the index under the composition of systems with the same symmetry in Eq. 3.73, we can deduce the index $\Theta$ by some algebraic manipulations. First, since $H^{(4)}_4$ has only $[X] = -2$ (see Table 3.1) and has MBS for both types, the contribution to the index from $[X]$ is $-1/2[X] \mod 2$. Then we take the Hamiltonian $2H^{(4)}_1 \oplus 2H^{(4)}_2 \oplus H^{(4)}_4$ (here and from now on we shorten the notation, $H^{(4)}_2 \oplus H^{(4)}_2 \equiv 2H^{(4)}_2$, and so on), in class $\chi^{(4)} = (4,0,0,0)$. This system has MBS in both types of disclinations, which implies a contribution to the index of $1/4$ in mod 2. Then we go back to $H^{(4)}_1$, which does not have MBS for any type, and solve for $1/4(Ch - 1/2[X] + x[M_1]) = 0 \mod 2$. Upon substitution of its invariants, we have $x = 1/4$, thus, there is a contribution to the index of $1/4[M_1] \mod 2$. Finally, we consider $H^{(4)}_1 \oplus H^{(4)}_2 \oplus H^{(4)}_3$, in class $\chi^{(4)} = (2,0,-1,1)$. This has MBS in both types. We solve for $x'$ in $1/4(Ch - 1/2[X] + 1/4[M_1] + x'[M_2]) \mod 2 = 1$ to find the contribution of $[M_2]$. This gives $x' = 3/4$.

Up to this point, only Hamiltonians that resulted in $G_{\nu} = (0,0)$ have been used. To find the influence of $G_{\nu}$ on the index let us consider $H^{(4)}_2$, which has $G_{\nu} = b_1 + b_2$, and MBSs at type-(1,0) disclinations, even though $1/4(Ch - 2[X] + [M_1] + 3[M_2]) = 0 \mod 2$. The reason that this MBS binds to the disclination is that the weak invariant $G_{\nu}$ is non-vanishing and the translation holonomy $T$ is odd for type-(1,0) disclinations. It is analogous to the topological index for MBSs at dislocations, with $T$ replacing the Burgers vector $B$. Joining these two pieces, and considering the linearity of the index on the Frank angle of Eq. 3.72, we find
Figure 3.15: Simulation of primitive model $H_2^{(4)}$ with the lattice configuration depicted in Fig. 3.14(a). (a) Density of states. The zoomed-in centered region of the insulating gap shows two zero-energy states with corresponding probability density functions exponentially localized around the disclination cores $O_1$ (b), and $K$ (c). The unit cell has $n = 20$ sites per side. The parameters used were $2u_2/\Delta = -u_1/\Delta = 1$.

Figure 3.16: Tight binding model $H_3^{(4)}$ with (a) type-(0,0) and (b) type-(1,0) disclinations, and model $H_4^{(4)}$ with (c) type-(0,0) and (d) type-(1,0) disclinations. Thick red dots in disclination cores are unpaired Majorana bound states.

\[ \Theta^{(4)} = \left[ \frac{1}{2\pi} \mathbf{T} \cdot \mathbf{G}_\nu + \frac{\Omega}{2\pi} (2C_h - 2[X] + [M_1] + 3[M_2]) \right] \mod 2. \] (3.75)

Crucially, the second term is an integer for all symmetry allowed choices of $\Omega$ because of the constraint in Eq. 3.29.

### 3.5.2 Twofold symmetry

Three of the four generators of $C_2$-symmetric superconductors also have $C_4$-symmetry. Indeed, the two spinless chiral $p_x + ip_y$ models $H_1^{(2)}$ and $H_2^{(2)}$, which are nothing but models $H_1^{(4)}$ and $H_2^{(4)}$, were already simulated with $\Omega = +\pi$ disclinations in the previous section. MBS were found only in the case of $H_2^{(2)}$ and even then only in the type-(1,0) disclination of Fig. 3.14(f). No MBS were found for the type-(1,1)
Table 3.2: Parity of the number of zero modes at disclinations for the \( C_n \) primitive models.

<table>
<thead>
<tr>
<th>symm.</th>
<th>disclination</th>
<th>primitive generators</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_4 )</td>
<td>Frank angle, type (-\pi/2, \text{type-(0,0)})</td>
<td>( H_1^{(4)} ) ( H_2^{(4)} ) ( H_3^{(4)} ) ( H_4^{(4)} )</td>
</tr>
<tr>
<td>( C_4 )</td>
<td>(-\pi/2, \text{type-(1,0)})</td>
<td>0</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>Frank angle, type (+\pi, \text{type-(0,0)})</td>
<td>( H_1^{(2)} ) ( H_2^{(2)} ) ( H_3^{(2)} ) ( H_4^{(2)} )</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>(+\pi, \text{type-(1,0)})</td>
<td>0</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>(+\pi, \text{type-(0,1)})</td>
<td>0</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>(+\pi, \text{type-(1,1)})</td>
<td>0</td>
</tr>
<tr>
<td>( C_6 )</td>
<td>Frank angle ( \pm \pi/3 )</td>
<td>( H_1^{(6)} ) ( H_2^{(6)} ) ( H_3^{(6)} )</td>
</tr>
<tr>
<td>( C_3 )</td>
<td>Frank angle, SC flux ( \pm 2\pi/3, \text{no extra flux} )</td>
<td>( H_1^{(3)} ) ( H_2^{(3)} ) ( H_3^{(3)} )</td>
</tr>
<tr>
<td>( C_3 )</td>
<td>( \pm 2\pi/3, \text{extra flux} )</td>
<td>0</td>
</tr>
</tbody>
</table>

To derive the index for the parity of MBS for \( C_2 \)-symmetric superconductors it will be convenient to define \( \Theta^{(2)} = \Theta_T^{(2)} + \Theta_R^{(2)} \), where \( \Theta_T^{(2)} = (1/2\pi)\mathbf{T.G}_\nu \) is the contribution to the index due to the translation part of the holonomy, and \( \Theta_R^{(2)} \) is the contribution due to the Chern and rotation invariants, which we are to determine. Consider \( H_1^{(2)} \), this generator has \( \mathbf{G}_\nu = (0,0) \) and therefore \( \Theta_T^{(2)} = 0 \) for all types of disclinations. This model does not have MBS for any disclination, so we require that \( \Theta_R^{(2)} = 0 \) for this set of invariants. Now consider \( H_2^{(2)} \) and \( H_3^{(2)} \), both of which have \( \mathbf{G}_\nu = (1,1) \), and therefore \( \Theta_T^{(2)} = 0 \) for type-(0,0) and type-(1,1) disclinations, but \( \Theta_T^{(2)} = 1 \) for type-(0,1) or type-(1,0) disclinations. For both models we observe MBS only for type-(0,1) and type-(1,0) disclinations, following the parity of \( \Theta_T^{(2)} \), thus, we require that \( \Theta_R^{(2)} = 0 \) for both of these sets of invariants as well. Finally, let us look at generator \( H_4^{(4)} \), which, unlike the previous three, breaks \( C_4 \) symmetry. This generator has \( \mathbf{G}_\nu = (0,1) \) and therefore \( \Theta_T^{(2)} = 0 \) for type-(0,0) and type-(1,0) disclinations and \( \Theta_T^{(2)} = 1 \) for type-(0,1) and type-(1,1) disclinations. This model has MBS precisely whenever \( \Theta_T^{(2)} = 0 \), therefore we require that \( \Theta_R^{(2)} = 1 \) for this set of invariants. Referring to Table 3.1 for the rotation invariants one can see that the four requirements for \( \Theta_R^{(2)} \) are met by the expression \( \Theta_R^{(2)} = 1/2(Ch + [X] + [Y] + [M]) \mod 2 \). Thus, appealing to the linearity of the index on the Frank angle.
Figure 3.17: Tight binding models $H_3^{(2)}$ (a-d) and $H_4^{(2)}$ (e-h) with $\Omega = +\pi$ disclinations. Disclinations are of type-(0,0) in (a,e), type-(1,0) in (b,f), type-(0,1) in (c,g), and type-(1,1) in (d,h). For $H_4^{(2)}$, gray lines serve only as a guide, and are oriented along the trivial (0,1) direction in a system with no disclinations, as in Fig. 3.7(c). Thick red dots in disclination cores are unpaired Majorana bound states.

of Eq. 3.72, the index for $C_2$-symmetric systems is

$$\Theta^{(2)} = \left[ \frac{1}{2\pi} \mathbf{T} \cdot \mathbf{G}_\nu + \frac{\Omega}{2\pi} (Ch + [X] + [Y] + [M]) \right] \mod 2. \quad (3.76)$$

The second term is always an integer due to the constraint in Eq. 3.30.

We finally point out that, since $C_4$-symmetric superconductors are also $C_2$-symmetric, a relation exists between the two indices when applying them to $\Omega = \pi$ disclinations. To see this, recall that the $C_2$ rotation invariants are related to the $C_4$ invariants by Eqs. 3.26 and 3.27. Thus the contribution of $2[X]^{(4)}$ inside the parenthesis of Eq. 3.75 splits into the contribution of $[X]^{(2)}$ and $[Y]^{(2)}$ in Eq. 3.76. Similarly, a contribution of $[M_1]^{(4)} - [M_2]^{(4)}$ in $\Theta^{(4)}$ maps to a contribution of $[M_1]^{(2)}$ in $\Theta^{(2)}$. We are left with a contribution of $4[M_2]$ in $\Theta^{(4)}$ that does not have a correspondence in $C_2$ rotation invariants, but this contribution is trivial, since $\Omega/2\pi(4[M_2]) = 0 \mod 2$ for $\Omega = \pi$ so there is no contradiction.

### 3.5.3 Sixfold symmetry

For $C_6$ symmetry the primitive models $H_1^{(6)}$ and $H_2^{(6)}$ were simulated by putting a triangular lattice on a torus geometry with periodic boundary conditions having two $\Omega = -\pi/3$ and two $\Omega = +\pi/3$ disclinations, as shown in Figs. 3.18(a). Since sixfold rotation symmetry exists only around vertices of the lattice, only one type of disclination can be considered, as shown in Figs. 3.18(b,c).
Figure 3.18: (a) Lattice cell of a $C_6$-symmetric lattice configuration having $\pm \pi/3$ disclinations. Periodic boundary conditions are imposed, by identifying edges on the unit cell marked with the same color of dashed lines. $O_{1,2}$ indicate centers of $-\pi/3$ disclinations. $K_{1,2}$ indicates centers of $+\pi/3$ disclinations. We also show examples of a (b) $-\pi/3$ disclination and a (c) $+\pi/3$ disclination.

Only 1st (2nd) nearest-neighbor hopping terms we used in $H_1^{(6)} (H_2^{(6)})$. The simulation parameters were $u_1/\Delta = 1$, $u_2 = 0$ for $H_1^{(6)}$, and $u_1 = 0$, $u_2/\Delta = 1$ for $H_2^{(6)}$. Unpaired MBS were found only for in $H_2^{(6)}$. Fig. 3.19 shows the density of states and the probability density functions for the zero-modes over a fraction of the lattice cell delimited by points $O_1$, $O_2$, $K_1$, and $K_2$ (notice that all disclination cores are covered by this region). The zoomed in region in Fig 3.19(a) shows the four zero-modes. The degeneracy at zero energy is lifted due to hybridization of the MBS wavefunctions due to the proximity of the disclination cores and it drops exponentially with increasing separation between the cores.

The third primitive model $H_3^{(6)}$ can be studied pictorially. Fig. 3.20 shows that this model harbors a MBS at its core, represented by the red open circle. The findings for all $C_6$ primitive models are summarized in Table 3.2.

As before, we can apply the linearity of the index under the composition of systems with the same symmetry in Eq. 3.73 to derive its form from this data. There is total freedom to choose linear combinations of Hamiltonians because there is no weak invariant in any $C_6$-symmetric superconductor. Let us start by taking $H_3^{(6)}$, which only has $[M] = -2$ and harbors a MBS. Thus, the contribution to the index is $-1/2[M]$ mod 2. Now, take $H_2^{(6)}$, and solve $x Ch - 1/2[M] = 1$ mod 2, to find a contribution of $1/2 Ch$ mod 2. Finally, take $H_1^{(6)}$, and solve $1/2 Ch - 1/2[M] + x'[K] = 0$ mod 2, which gives $x' = 0$, that is, the invariant $[K]$ does not contribute to the index. The topological index for $\Omega = \pm \pi/3$ disclinations is then given by $\Theta = 1/6(3Ch - 3[M])$ mod 2. The linearity of the index on the Frank angle of Eq. 3.72 implies that the topological index for a generic $C_6$ disclination with Frank angle $\Omega$ is

$$\Theta^{(6)} = \frac{\Omega}{2\pi} (3Ch - 3[M]) \mod 2.$$ (3.77)
Figure 3.19: Simulation of primitive model $H_2^{(6)}$ with the lattice configuration depicted in Fig. 3.18. (a) Density of states. The zoomed-in centered region of the insulating gap shows four zero-energy states with corresponding probability density functions centered at negative disclinations $O_1$, $O_2$ (b,c), and positive disclinations $K_1$, $K_2$ (d,e). The unit cell has $n = 24$ sites per side. The parameters used were $u_1/\Delta = 0$, $u_2/\Delta = 1$. The splitting of the states near zero energy is due to the finite size of the lattice.

Figure 3.20: Tight binding model $H_3^{(6)}$ with a $\Omega = -\pi/3$ disclination. The thick red dot in disclination cores is an unpaired Majorana fermion.

The index is always an integer because of the constraint in Eq. 3.31 on the Chern and rotation invariants. There is no translation term since the weak-invariant always vanishes for $C_6$ symmetry.

### 3.5.4 Threefold symmetry

For superconductors $H_1^{(3)}$ and $H_2^{(3)}$, which are $C_6$-symmetric, the index $\Theta^{(6)}$ predicts no MBS in $\Omega = 2\pi/3$ disclinations. To corroborate this, and to investigate the third primitive generator $H_3^{(2)}$, which breaks $C_6$ symmetry, all three models were simulated by putting their triangular lattices on a torus. This time, only one $\Omega = -2\pi/3$ disclination and one $\Omega = +2\pi/3$ disclination were necessary to compensate curvature, as shown in Fig. 3.21(a). Just as in the $C_6$ case, $G_v = 0$, and only disclinations centered at vertices need to be
Figure 3.21: (a) Lattice cell of a $C_3$-symmetric lattice configuration having $\Omega = \pm 2\pi/3$ disclinations. Periodic boundary conditions are imposed by identifying edges on the lattice cell marked with the same type of dashed lines. $O$ indicates the center of the $\Omega = -2\pi/3$ disclination, and $K$ indicates the center of the $\Omega = +2\pi/3$ disclination. We show examples of a (b) $\Omega = -2\pi/3$ disclination and a (c) $\Omega = +2\pi/3$ disclination.

Figure 3.22: Simulation of primitive model $H_1^{(3)}$ with the lattice configuration depicted in Fig. 3.21. (a) Density of states showing two zero-energy states with corresponding probability density functions centered at the $\Omega = -2\pi/3$ disclination core $O$ (b), and at the $\Omega = +2\pi/3$ disclination core $K$ (c). Superconducting fluxes of $\pm 8\pi/3$ bind the disclinations. The unit cell has $n = 18$ sites per side. The Hamiltonian parameters were set to $u_1/\Delta = 1$ and $u_2/\Delta = 0$.

Simulations indicated that no MBS exist for any of the three models. However, when fluxes of $\pm \Omega \pm 2\pi$ were bound to the disclinations with Frank angles of $\pm \Omega$ respectively, MBS appeared in all models, and in all disclinations. Fig. 3.22 shows simulation results for $H_1^{(3)}$ with an extra quantum of flux added.

The findings for all $C_3$ primitive models are summarized in Table 3.2.

The results indicate that the index does not depend on either $[K^{(3)}]$ or $[K']^{(3)}$, which is expected since the index for $C_6$-symmetric systems was independent of $[K]^{(6)}$. This, in addition to the information summarized in Table 3.2 leads to the index

$$\Theta^{(3)}(\Omega) = \left(\frac{\Omega}{2\pi} + 1\right) 3Ch \mod 2 \quad (3.78)$$

for $0 \leq \Omega \leq 4\pi$. Notice that, unlike the cases treated before, $\Omega$ here accounts for the superconducting flux, and not the classical Frank angle of the disclination. Both can either be the same or differ by an extra flux.
quantum of $2\pi$, as discussed in Sec. 3.4. In the case of binding extra quanta of flux to disclinations in lattices where the order of rotation $n$ is even, a different rotation operator is associated, thus changing the rotation invariants in accordance with Eq. 3.21. In any case, the result amounts to an inversion of the parity of MBS whenever the Chern invariant is odd, which resembles the usual result in Ref. [95] for the parity of MBS in quantum vortices.

### 3.6 Disclination and corner Majorana bound states in Strontium Ruthenate Sr$_2$RuO$_4$

The $\mathbb{Z}_2$ topological index $\Theta$ that counts the MBS number parity at a disclination applies to all two-dimensional gapped crystalline superconductors described by a mean field BdG Hamiltonian. In this section, we predict the existence of disclination or corner-bound Majorana zero modes in Strontium Ruthenate. This material has a layered perovskite structure and can be approximated by a quasi-two-dimensional theory with a fourfold lattice rotation symmetry. It is an unconventional superconductor when $T \lesssim 1.5$K, and its superconducting order parameter shows spin-triplet $p$-wave characteristics, which is odd under time reversal and parity [134, 135, 136, 137]. The exact nature of the pairing order has been controversial. It was postulated to be a chiral $p_x + ip_y$ state [138] however the expected edge current [139, 140] was not detected with the predicted magnitude [141, 142, 143]. The triplet pairing was later theoretically suggested by Raghu-Kapitulnik-Kivelson in Ref. [144] to be non-chiral and predominantly generated from the quasi-one-dimensional $d_{xz}$ and $d_{yz}$ bands instead of the two-dimensional $d_{xy}$ band. More recently there is STM evidence supporting the quasi-1D non-chiral nature of the material. [145] In recent work, Majorana bound states were predicted to be present on linked dislocation lines in the 3D material due to the non-trivial $\mathbb{Z}_2$ weak invariants $G_{\nu} = b_1 + b_2$ [81]. Here we discuss the MBS number parity at disclination and/or corner defects in Sr$_2$RuO$_4$ using the quasi-one-dimensional model proposed in Ref. [144].

The electronic band theory of the material at the Fermi energy is controlled by the $t_{2g}$ orbitals of Ruthenium. In the normal metallic phase, the quasi-two-dimensional $d_{xy}$ band forms a Fermi circle while the quasi-one-dimensional $d_{xz}$ and $d_{yz}$ bands give horizontal and vertical Fermi lines [see Fig. 3.23(a)]. We will focus only on the spin triplet superconductivity of the $d_{xz}$ and $d_{yz}$ bands, which were predicted by Ref. [144] to be the dominant superconducting pairing, and we will ignore the effects of spin-orbit coupling. Because of the quasi-1D nature, each band is physically identical to an array of weakly coupled electron wires, which, in the presence of triplet superconductivity, become the Kitaev $p$-wave chains [93]. The $d_{xz}$ and $d_{yz}$ arrays are stacked perpendicular to each other and form a fourfold rotation symmetric system. This
Figure 3.23: Corner-localized Majorana bound states in the normal metallic phase of \( \text{Sr}_2\text{RuO}_4 \). (a) Schematics of the (unhybridized) Fermi surfaces of the normal metallic phase. In the Raghu-Kapitulnik-Kivelson state, the \( d_{xy} \) and \( d_{yz} \) bands (horizontal and vertical red lines) are responsible for superconductivity while the \( d_{xy} \) one (dashed blue circle) is ignored \[144\]. (b) Tight binding limit of the superconducting \( d_{xz} \) and \( d_{yz} \) bands. Dashed lines on the edges represent allowed perturbations that will gap the edge Majorana modes and leave an unpaired MBS (red dot) at each corner.

model of \( \text{Sr}_2\text{RuO}_4 \) is therefore topologically equivalent to the Hamiltonian \( H^{(4)}_3 \) in Eq. 3.41 with non-zero nearest neighbor hopping \( u_1 \), but vanishing next nearest hopping \( u_2 \). This is pictorially represented by the Majorana tight binding model in Fig. 3.7 or 3.23(b). In reality, there are weak inter-wire couplings and spin-orbit coupling which hybridize different orbitals (both the order of magnitude of 10% of \( u_1 \)). The topology of the BdG Hamiltonian \( H^{(4)}_3 \) is insensitive to these perturbations although in the real material spin-orbit coupling would be essential in determining the dominant superconducting order.

With this description, \( \text{Sr}_2\text{RuO}_4 \) does not carry a chiral edge mode. However it carries a non-trivial weak topology with index as in Eq. 3.33 as well as rotation symmetry protected invariants shown in Table 3.1. As a result, the \( \mathbb{Z}_2 \) index in Eq. 3.75 predicts an odd MBS number parity at a type-(0, 0) 90° disclination and an even parity at a type-(1, 0) one [see Fig. 3.16(a,b)]. Since MBS always come in pairs, the periphery of the \((0, 0)\)–disclination system must also carry an odd number of Majorana modes. However, the non-trivial weak topology implies the existence of an additional non-chiral gapless channel along an edge that can couple to the corner states. Luckily, surface perturbations can open a gap for the non-chiral channel, e.g., a density wave perturbation [dashed lines in Fig. 3.23(b)], which will leave an odd number of MBS at each corner (represented by red dots). Unlike disclination MBS which are protected by the bulk energy gap, corner MBS are only weakly protected as they can escape through accidental or topological gapless edge channels. We note that since \( \text{Sr}_2\text{RuO}_4 \) is really a 3D material, the existence of MBS implies the existence of a channel of chiral Majorana modes propagating on disclination/corner lines in the 3D sample. We also need to restore the spin degree of freedom which implies that there will be pairs of MBS, one for each spin which could be coupled via the spin-orbit coupling.
3.7 Summary

The primary goal of this work was to provide a topological classification for 2D superconductors with discrete rotation symmetry as well as index theorems that determine the parity of Majorana bound states in composite defects composed of fluxes, dislocations, and disclinations. We have found the classification to be quite rich and varied across the different $C_n$ rotation symmetries. Since most crystalline systems exhibit some type of 2D rotation symmetry, the results of this work can be applied to a broad class of crystalline superconductors. We found that even in systems with an even integer or vanishing Chern number, disclination defects can bind an odd number of Majorana bound states. There are even cases when both the Chern number and weak invariants are trivial and disclinations still bind an odd number of Majorana modes due to topological rotation invariants.
In this dissertation, we have extended the theory of polarization in crystalline insulators to account for higher electric multipole moments. We found that crystalline insulators can host quadrupole moments in 2D and octupole moments in 3D.

One of the most exciting results of our work is that in the presence of symmetries, multipole moments can take quantized values. Insulating phases realizing the quantized value are recognized to have a topological character protected by the enforced symmetries. However, the properties of the quadrupole and octupole topological phases are remarkable in the sense that, instead of exhibiting gapless states on the boundary, these phases have gapped boundaries, which are themselves nontrivial SPT phases of lower spatial dimension. This defies the conventional idea of topological phases of matter as phases with a gapped, featureless bulk that, because of their topological nature, require the existence of gapless states on the boundary. Instead, the picture here is similar to the concept in 3D topological phases that a gapped, symmetry-preserving surface cannot be trivial and must have topological order [88, 89, 90, 91, 92]. A similar structure follows in the case of the octupole moment; a bulk octupole SPT insulator in 3D generates corner-localized mid-gap bound states, as well as 6 quadrupole SPT phases on its 2D surfaces, and 12 dipole SPT phases on its 1D hinges, all of which converge at the 3D corners. Hence, the quadrupole and octupole phases represent a new mechanism for the realization of SPT phases, i.e., surface SPTs.

This then offered us the possibility of exploring similar realizations in other phases of matter. Particularly, we explored 2D topological superconductors, in which zero-dimensional corner-localized Majorana bound states are the natural boundary manifestation. To study the role of defects, we systematically classified time-reversal breaking topological superconductors in 2D, and built index theorems for the existence of Majorana bound states at the cores of topological defects, which include dislocations, disclinations, and vortices.

Following this line of reasoning, our work can naturally be extended to the characterization of other 2D or 3D systems exhibiting edges/surfaces that are gapped fermionic/bosonic SPTs or $\mathbb{Z}_n$ parafermion chains. The study of these systems has already begun, not only for the existence of zero-dimensional states.
localized on corners of 2D crystals [146, 147, 148, 149, 150], but also for one-dimensional chiral or helical states localized at hinges of crystals in 3D [151, 152, 153], and not only in electronic crystals, but also beyond [154, 155, 64, 156].
Appendix A

A metamaterial analog of the quadrupole topological insulator

In this appendix, I summarize the work published in Ref. [155] on the construction of a metamaterial analog of the quadrupole model in Eq. 2.155, with a lattice shown in Fig. 2.20. The construction of metamaterial analogs of electronic systems is a growing field. Metamaterial analogs of the quantum Hall and quantum spin Hall topological insulators have previously been implemented in phononic and photonic systems [157, 158, 159, 160].

We focus on the detection of the zero-energy corner-localized modes because they can provide direct spectroscopic evidence for the existence of the non-trivial quadrupole topological phase. Furthermore, we provide evidence that these corner modes are not due to surface effects, but are required by the topological bulk phase.

The metamaterial in question is composed of coupled microwave resonators in a square lattice of unit cells. Each unit cell is composed of four identical resonators, as shown in Fig. A.1. Each plaquette contains a single negative coupling term (dashed lines in the schematic of Fig. A.1(a) which amounts to the generation of a synthetic magnetic flux of \( \pi \) puncturing the plaquette. The existence of this non-zero flux opens both the bulk and edge energy gaps, which are necessary to protect the corner-localized mid gap modes.

Each resonator is implemented using an \( H \)-shaped microstrip transmission line that has a fundamental resonance at \( f_0 = 2.08 \text{ GHz} \), having linewidth \( \sim 20 \text{ MHz} \), with a spatial voltage distribution as illustrated in Fig. A.1(a). At the center of the cross piece lies a voltage node while each end-point of the \( H \)-shape is a quarter-wavelength from the center and is, therefore, an anti-node. Adjacent tips of the \( H \) are separated by a half-wavelength and thus differ in phase by \( \pi \) rad, and the pinched-in ends are designed to bring the anti-nodal points having opposing phase physically close together. To produce the quadrupole topology, in each plaquette we arrange three couplings as positive and one coupling as negative as shown in Fig. A.1(a).

We first experimentally confirm that a \( \pi \) flux threads each plaquette by examining the limiting cases of \( \lambda \to 0 \) and \( \gamma \to 0 \). This experimental verification of \( \pi \) flux of the isolated unit cell plaquettes as shown in Fig. A.1(b), where we show the measured power absorptance spectrum (the ratio of absorbed power to incident power). As predicted, we find two pairs of nearly degenerate modes separated by \( 2\sqrt{2}\gamma \approx \)
Figure A.1: **Unit cell of the microwave quadrupole lattice.** (a) A unit cell of the quadrupole topological insulator, composed of four capacitively coupled H-shaped microstrip resonators, each having a fundamental mode at 2.08 GHz as illustrated (colors represent voltage amplitude). The coupling between R4 and R1 is set as negative, as shown in the detailed schematic, in order to produce $\pi$ flux through the unit cell plaquette. (b) Eigenmodes (presented as phasor diagrams: circle diameter corresponds to the magnitude of the resonator excitation, the line corresponds to the phase) when driving R4 (left) and when driving R3 (right). (c) Resonance frequencies for modes in (b).

The spatial distribution of the lower pair of modes is measured through the voltage amplitude and phase response at each resonator within the plaquette when either resonator R3 or R4 is stimulated. The zero amplitude found in the resonators diagonal to the resonator being stimulated confirms the destructive interference caused by the $\pi$ flux between counter-circulating paths around the plaquette.

An array of the lattice of resonators having $5 \times 5$ array of unit cells, as shown in Fig. A.2(a). It has a coupling ratio of $\lambda/\gamma \approx 4.3$. The average absorptance across the entire array is shown in Fig. A.2(b). Three spectral bands are identifiable: broad lower and upper bands (purple and pink, respectively) separated by a bandgap, and a narrow band of modes near the center of the bandgap (cyan). The spatial distributions of each of these bands, obtained by summing over each band indicated in Fig. A.2(b), are shown in Figs. A.2(c). We find that, as expected from the analysis in Section 2.6.4, modes in the lower and upper bands are predominantly localized on the bulk and edge resonators. The modes in the center of the bandgap, associated with corner charges in the case of an electrical insulator, are highly localized on the corner resonators only. Furthermore, the measured spectra of the individual corner resonators confirm that each corner supports only a single mid-gap mode, as shown in Fig. A.2(d).

Due to parasitic couplings and possibly disorder in the array the measured spectrum is asymmetric with respect to its mid-gap point. There are two main sources of disorder: (i) systematic differences in the capacitive loading of resonators within the array, and (ii) random disorder due to small manufacturing variations in the capacitance of the discrete coupling capacitors. Despite such disorder, the robust spectral
Figure A.2: **Demonstration of microwave quadrupole topological insulator.** (a) Photograph of the experimental array of coupled resonators that form the quadrupole lattice. The array has $5 \times 5$ unit cells. (b) Normalized average absorptance spectrum (ratio of absorbed microwave power to incident power) of all the resonators in the array. We observe two large bands (purple and pink) separated by a bandgap containing in-gap modes (cyan). (c) Spatial distribution of absorptance summed over the lower frequency band (left) in-gap band (center) and upper band (right). (d) Individual absorptance spectra of the corner resonators. Each corner resonator only supports a single mode.
Figure A.3: Experimental test of topologically protected corner states during edge deformation. (a) The entire array is initially set in the topological phase with $\lambda/\gamma = 4.3$, with the exception of the unit cells in the bottom row, which are brought into the trivial regime with $\lambda_e/\gamma_e = 1/4.3$. (b) Frequency response of the lowest two rows of unit cells. (c) Measured spatial distribution of modes. The mid-gap modes localize on the new corners of the quadrupole topological phase.

features of the quadrupole topological insulator remain, e.g. the spectral bands are gapped, with only 4 resonances at positions close to mid-gap.

To demonstrate that the corner-localized modes are not the result of local effects particular to the physical edges of the array, we tune the unit cells on the lowest row from the topological regime ($\gamma < \lambda$) to the trivial regime ($\gamma > \lambda$). This experiment begins with the entire array in the original topological phase ($\lambda/\gamma \approx 4.3$) as shown previously in Fig. A.2. Then, by replacing the coupling capacitors within the network, we adjust the coupling rates on the bottom row of unit cells to be in the ratio $\lambda_e/\gamma_e = 1/4.3$. Although the physical bottom edge of the array is now in the trivial regime, the corner modes are not destroyed but simply recede to the new topological phase boundary. This experimental observation confirms that the corner modes are not just a surface artifact, but rather they are a unique manifestation of the bulk quadrupole topological phase. In contrast, if the corner modes were generated from localized defects on the corners, or even if they arose as the end-states of edge-localized 1D topological dipole insulators, the mid-gap modes would disappear during the edge deformation.
Appendix B

Topological protection of corner modes in photonic crystals

In this appendix, I summarize the work published in Ref. [154] on the experimental observation of mid-gap modes localized at corners of photonic topological crystals. The lattice used here is the same as that of model $H_3^{(6)}$ in Section 3.3. However, the physical implementation and nature of the boundary signatures are radically different. We use an array of evanescently-coupled waveguides written into fused silica by the femtosecond direct laser writing technique [161]; the geometry of the lattice we employ [shown in Figs. B.1(a-f)] is a modified version of the lattice shown in Fig. 3.7(d) in the context of topological superconductors, where the corner-localized mid-gap modes correspond to Majorana bound states.

Each waveguide in the lattice supports a single bound mode. The equation governing the diffraction of light through the structure is:

$$i \frac{d}{dz} \psi_i(z) = - \sum_j c_{ij}(\lambda) \psi_j(z), \hspace{1cm} (B.1)$$

where $z$ is the distance along the waveguide axis and $\psi_i$ is the amplitude associated with the $i^{th}$ mode. The coupling constants $c_{ij}(\lambda)$ between waveguides labelled $i$ and $j$ are wavelength ($\lambda$) dependent. In the transverse plane, the waveguide array has $C_6$ symmetry as shown in Fig. B.1. The primitive lattice is triangular and each unit cell has six waveguides. Neighboring waveguides within the unit cell are separated by a distance $s$ (a parameter that we tune in the experiment), and the lattice constant is $L = 60 \mu m$. The ratio between these two lengths $L$ and $s$ allows tuning between two topologically distinct gapped phases. For $L/s > 3$ this structure is topologically trivial, at $L/s = 3$ it is gapless, and for $L/s < 3$, it is topologically nontrivial.

The corresponding lattices in the approximation of nearest-neighbor coupling are shown in Fig. B.1 (d-f). The unit cell (marked in green) has six waveguides, and we distinguish two types of coupling terms: those between waveguides within a unit cell, of strength $c_{\text{int}}$, and those between waveguides belonging to neighboring unit cells, of strength $c_{\text{ext}}$. The Bloch Hamiltonian for these lattices is

$$h(k) = c_{\text{ext}} h_{\text{ext}}(k) + c_{\text{int}} h_{\text{int}}, \hspace{1cm} (B.2)$$

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Figure B.1: $C_6$ symmetric photonic lattices and band structures belonging to different topological phases. Trivial phase (left column) with $L/s = 3.53$, critical phase at $L/s = 3.00$ (center column), and topological phase with $L/s = 2.61$ (right column). (a-c) Cross-sectional microscope images of the input facet of the photonic waveguide lattices. (d-f) Diagrams of the lattices. Green hexagon in (d) delimits a unit cell. Black (red) lines represent intra-cell (extra-cell) couplings of strength $c_{\text{int}}$ ($c_{\text{ext}}$) in the tight-binding approximation. The color of the waveguides represents their sublattice. The structural parameters $L$ and $s$ are labeled in (d); they are the separation between hexagons and the distance from the center of the hexagon to one of its component waveguides, respectively. (g-i) Band dispersion calculated using the tight-binding approximation for a ribbon configuration with closed boundaries in the $x$ direction and open in the $y$ direction (thus, having armchair edges). The mid-gap bands in (i) (dashed light-blue lines) have (nonprotected) eigenstates localized at edges.

where $h_{\text{ext}}(k) = \oplus_{i=1}^{3} [\cos(k \cdot a_i)\sigma_x + \sin(k \cdot a_i)\sigma_y]$ is due to couplings between waveguides of neighboring unit cells, and $h_{\text{int}}$ is a matrix with entries $[h_{\text{int}}]^{mn} = 1$ for nearest-neighbor waveguides $m$, $n$ within the same unit cell, and 0 otherwise. Here $a_1 = (1, 0)$, $a_{2,3} = (\pm 1/2, \sqrt{3}/2)$ are primitive lattice vectors, and the basis of states in the matrices are the six internal degrees of freedom in the unit cell [see Fig. B.1(d) for numbering].

These lattices have chiral (i.e. sublattice) symmetry. To see this, let us first identify the existence of two sublattices, each corresponding to sites having the same color in Fig. B.1(d-f). Chiral symmetry exists when the couplings between sites on the same sublattice are vanishing. This is a good approximation for our system as the coupling terms $c_{ij}(\lambda)$ decrease exponentially with separation between waveguides for all
wavelengths \( \lambda \) in our range of interest, and thus, couplings between waveguides further apart than nearest-neighbors are increasingly exponentially suppressed. TR-invariant photonic systems belong to classes AI or BDI in the periodic 10-fold classification of topological phases [23, 24], and in two dimensions none of these classes exhibit topological phases [162]. Thus, any topological protection will have to necessarily arise from the existence of extra symmetries, e.g., discrete translation or point-group symmetries. This is the case in this model. In addition to chiral symmetry, it has \( C_6 \) rotation symmetry. Following the classification procedure based on point group representations of the Hamiltonian below the gap as in Chapter 3, but imposing restrictions on the invariants due to TRS instead of those due to particle-hole, the bulk topology of the tight-binding Hamiltonians in class AI under \( C_6 \) symmetry is classified by

\[
\chi^{(6)} = ([M], [K]), \tag{B.3}
\]

where \([M] \in \mathbb{Z}\) and \([K] \in \mathbb{Z}\) are \( C_2 \) and \( C_3 \) topological invariants, respectively. They are defined as follows,

\[
[M] = \# M_1 - \# \Gamma_1^{(2)}, \quad [K] = \# K_1 - \# \Gamma_1^{(3)}, \tag{B.4}
\]

where \( \# M_1 \) (\( \# \Gamma_1^{(2)} \)) is the number of states below the gap with \( C_2 \) rotation eigenvalue +1 at the \( M \) (\( \Gamma \)) point of the BZ, and \( \# K_1 \) (\( \# \Gamma_1^{(3)} \)) is the number of states below the gap with \( C_3 \) rotation eigenvalue +1 at the \( K \) (\( \Gamma \)) point of the BZ. The invariant \([M] ([K])\) is a measure of the difference in the \( C_2 \) (\( C_3 \)) rotation representations that the subspaces of negative energy states take at \( h(M) h(K) \) and \( h(\Gamma) \).

In our system, the \( C_3 \) rotation operator and the chiral operator commute. This implies that \([K] = 0\) for all ratios of \( c_{\text{int}}/c_{\text{ext}} \). Since, on the other hand, the \( C_2 \) rotation operator and the chiral operator do not commute, the invariant \([M]\) is not restricted to zero. It takes the values

\[
[M] = \begin{cases} 
0 & \text{if } |c_{\text{int}}/c_{\text{ext}}| > 1 \\
2 & \text{if } |c_{\text{int}}/c_{\text{ext}}| < 1.
\end{cases} \tag{B.5}
\]

Equivalently, \([M] = 2\) for \( L/s < 3 \) and \([M] = 0\) for \( L/s > 3 \). In the \([M] = 0\) phase, our photonic lattice can be adiabatically connected to a photonic lattice having no inter-cell coupling (i.e., the “atomic limit”, in an analog atomic lattice) without closing the energy gap. This is the trivial phase. When \([M] = 2\), such an adiabatic connection is not possible unless we close the bulk energy gap (or break the \( C_2 \) symmetry, which is forbidden in this context). Thus, \([M] = 2\) signals a different phase when \( C_6 \) (and hence \( C_2 \)) is present.
Figure B.2: (a) DOS of the lattice in the trivial phase ($L/s = 3.53$). (b) DOS of lattice in the topological phase ($L/s = 2.61$). Inset: Enlarged DOS around $\beta = 0$. Inset labels correspond to the states shown in (c-e). (c) Combined LDOS of the six topologically-protected zero modes. (d) Combined LDOS of the twelve edge modes. (e) Combined LDOS of the twelve trivial corner modes.

One observable consequence of the nontrivial topology is the existence of energy-degenerate corner-localized topological bound states. This is shown in Fig. B.2. Only bulk bands exist in the trivial phase, whereas three types of boundary modes emerge in the topological phase: protected topological zero-modes on the corner unit cells [Fig. B.2(c)], gapped edge modes [Fig. B.2(d)], and gapped corner modes [Fig. B.2(e)]. Crucially, although both the topological corner modes (also called “zero modes”) and the trivial corner modes are localized together at the corners, they do not hybridize to open a gap. Doing so would require breaking chiral symmetry. Indeed, out of the initial three topological corner modes per corner unit cell, two of them hybridize as chiral-symmetric partners. This results in the gapped trivial corner modes. The topological corner modes, on the other hand, remain at $\beta = 0$. The zero-modes are eigenstates of the chiral operator, with chiral eigenvalues as indicated by the signs in Fig. B.2(c).

The existence of the bound defect modes in the presence of chiral symmetry is indicated by a topological index $N \in \mathbb{Z}$ that captures the interplay between the topology of the bulk Hamiltonian and the topological structure of the defect [162]. The chiral topological indices $N$ for each corner indicate the number of protected modes at $\beta = 0$ energy at that corner and are robust in the presence of disorder. If the disorder breaks $C_6$ (or even just $C_2$) but preserves chiral symmetry (e.g., if the disorder is due to small imperfections in the positioning of the waveguides), the topological corner modes will still be localized and pinned at $\beta = 0$.

To probe the relevant modes, a beam was launched at the input facet of the photonic lattice through
Figure B.3: Experimentally measured diffracted light at the output facet of the photonic crystal. (a) Trivial phase \( L/s = 3.53 \). (b) Critical point \( L/s = 3 \). (c) Nontrivial phase \( L/s = 2.61 \). A color bar is presented on the right side of (a), giving the light intensity at the output facet on a relative scale. The wavelength of the optical field is set to \( \lambda = 1450 \) nm. White arrows indicate the position of light injection.

Figure B.4: Direct excitation of a zero mode using an auxiliary waveguide weakly coupled to the system. (a) Microscope image of the waveguide array used in the experiment, including the auxiliary waveguide; (b) Experimental excitation of an optical zero mode at \( \lambda = 1650 \) nm. Dashed circles mark the positions of the waveguides.

a lens-tipped fiber, which allows us to couple the beam into a single waveguide. In Fig. B.3, diffracted light is shown emerging from the output facet for three different wavelengths and in three different cases: trivial phase [Fig. B.3(a)], critical phase-transition point [Fig. B.3(b)], and topological phase [Fig. B.3(c)]. For the trivial phase, the light injected into a corner simply diffracts into the bulk. For the critical phase, spreading easily occurs because there is no bandgap at all. On the other hand, in the topological phase, light is confined close to the corner at which the light is injected.

In order to demonstrate that the corner mode lies exactly at mid-gap, we use a modification of a previously developed technique [163] to excite waveguide array modes at a particular energy, which consists of creating an auxiliary waveguide sufficiently far away from the lattice that it is weakly coupled to it, as shown in Fig. B.4. This waveguide injects light into the system at exactly the energy of its bound mode. Since it is identical to every other waveguide in the system, the energy of the light injected into the main array is zero (precisely at mid-gap). As shown in Fig. B.4(b), we observe that in the topological array precisely the zero mode is excited [compare the excited pattern with the local density-of-states of the zero modes shown in Fig. B.2(c)].
Zero-dimensional modes have been observed in photonics, but they come as the boundary modes of one-dimensional (1D) topological systems [164, 165, 166, 167, 168, 169]. The zero-dimensional modes shown in this appendix suggest a much wider range of platforms over which these modes can be realized. Possible applications that employ confined cavity modes in such lattice-based platforms include enhanced coupling to quantum emitters [170], low-threshold lasing [171] and enhanced nonlinearity for supercontinuum generation [172].
References


