Spatially-protected Topology and Group Cohomology in Band Insulators

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Abstract

This thesis investigates band topologies which rely fundamentally on spatial symmetries. A basic geometric property that distinguishes spatial symmetry regards their transformation of the spatial origin. Point groups consist of spatial transformations that preserve the spatial origin, while un-split extensions of the point groups by spatial translations are referred to as nonsymmorphic space groups. The first part of the thesis addresses topological phases with discretely-robust surface properties: we introduce theories for the \( C_{nv} \) point groups, as well as certain nonsymmorphic groups that involve glide reflections. These band insulators admit a powerful characterization through the geometry of quasimomentum space; parallel transport in this space is represented by the Wilson loop. The non-symmorphic topology we study is naturally described by a \textit{further} extension of the nonsymmorphic space group by quasimomentum translations (the Wilson loop), thus placing real and quasimomentum space on equal footing – here, we introduce the language of group cohomology into the theory of band insulators. The second part of the thesis addresses topological phases without surface properties – their only known physical consequences are discrete signatures in parallel transport. We provide two such case studies with spatial-inversion and discrete-rotational symmetries respectively. One lesson learned here regards the choice of parameter loops in which we carry out transport – the loop must be chosen to exploit the symmetry that protects the topology. While straight loops are popular for their connection with the geometric theory of polarization, we show that bent loops also have utility in topological band theory.
I have always enjoyed reading this section in the work of others, even where I have no intelligent opinion in the scientific merit of said work. The nature of this thesis demands I acknowledge the people who have steered, nudged, inspired, or directly pushed me into the fire. Despite my omission of unrelated joys, there are still many people to thank.

I recollect a gathering with Andrei and Emil. Emil asked semi-rhetorically, “What problem shall we solve today?” Andrei replied fervently, “Everything.” I hope to have imbibed some of his gung-ho, take-no-prisoner ambition. His standard for clarity and rigor in thinking and writing shall be my standard. He taught me that coincidences were symmetries waiting to be unmasked – this thesis describes our unmasking.

Chen Fang listened patiently to many of my errant speculations, until some of them eventually struck home. To him I owe the debt of levelling me up from slaying rats in the basement, and for accelerating my productivity. His experience in band theory steered many conversations into discoveries, and we drank together the wine of shared ideas, and sometimes just plain wine and too much of it. Our musings in wintery Aspen, while soaking in mountain-top, open-air jacuzzis, birthed Chap. 3.

My unlikely partnership with Wang Zhijun proved instrumental to this thesis. He arrived in Princeton with big dreams but little English – our mode of communication was at first completely mathematical. Nevertheless, his insights in material chemistry complemented my abstract, group-theoretical perspective. He found the KHgX material class whose true beauty was veiled to us in the months that we prodded and probed. After a chance dinner at Szechuan House, he suggested that our hourglass fermion might be robust but didn’t
know why; in completing his thought I (or we!) discovered the hourglass-zigzag topology, which underlies Chap. 4.

I arrived in Princeton at Daniel Arovas’ insistence, and in the ensuing five years he would frequently descend at Princeton as a whirlwind, whipping out his brand of wit and physical intuition. When I professed to being lost in in existentialist crisis, he threatened to put a fork through my hand. He introduced me to elementary band representations, which sparked an insight detailed in Part IV. His support throughout my career has been tremendous.

Nicolas Regnault is a giant. When he flexes, beautiful numerics stream out. Our conversations flow from parafermions to practical know-how, e.g., how to find a job without despairing, and how to sensitively acknowledge collaborators in talks – by joking at the expense of the French. I partook so much of his intelligence, compassion and humor.

I have had the immense pleasure of being the resident shrink for band-topological advice. Belopolski often bursts through my office door to bounce off his latest ideas. He writes frenetically on the board, then peers back at me to register my reactions. Since my reactions are often not forthcoming, an awkward silence ensues whereupon my rising impatience chokes me to further silence. Many episodes occur in this fashion. I will miss many things about Belopolski, but I will not miss that searching look. Some semblance of ideas seep through, and it is still hopeful that one of them will bear fruit. Among proven collaborations with more-serious experimentalists, Nasser sold me a mystery whose definitive solution eluded me, though I have my speculation. Our joint exploration of the Cerium monopnic-tides uncovered a beautiful example of band-theoretical holography. Bismuth christened me to nature’s fold, and instilled in me a deep-seated belief in band theory. Here marked my first rewarding partnership with an experimentalist, Ilya Drozdov, with whom many nights were spent understanding the scattering of Bloch waves.
My parents, Rugai and Connie, carried my burdens and actualized my evanescent dream.

My sisters, Charmelia, Nina, Sasha, Marcia, and Laetitia, withstood my long absences.

I wish it were not so.

To Katie, with whom I shared the first tentative steps.

I bear you, now, sure-footed.
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Part I

Introduction

Insulating phases are deemed distinct if they cannot be connected by continuous changes of the Hamiltonian that preserve both the energy gap and the symmetries of the phase; in this sense we say that the symmetry protects the phase. Distinct phases have strikingly different properties – some nontrivial phases are characterized by robust boundary modes which are particularly accessible through experimental techniques, e.g., STM and ARPES. For many well-known topological insulators, the existence of boundary bands is in one-to-one correspondence with the topology of the bulk wavefunctions. [1] Examples include the Chern insulator [2] and the quantum spin Hall insulator [3]; these non-interacting insulators fall under ten well-known symmetry classes which are distinguished by time-reversal, particle-hole and chiral symmetries. [4] Given the completeness of this classification, attention has shifted to identifying topological phases which rely on other symmetries. [5]

The symmetries which are ubiquitous in condensed matter are the crystal space groups. A basic geometric property that distinguishes these symmetries regards their transformation of the spatial origin: rotations, inversions and reflections preserve the origin, while screw rotations and glide reflections unavoidably translate the origin by a fraction of the lattice period. [6] Point groups consist of transformations that preserve the origin, and the 73 symmorphic space groups are the obvious combinations of point groups with spatial
translations. Here, ‘obvious’ means a semidirect product of the two groups, which is also referred to as a split extension of the point group by spatial translations; less obvious are the un-split extensions, which comprise the 157 nonsymmmorphic space groups. No origin exists that is simultaneously preserved by all symmetries in a nonsymmmorphic group, modulo lattice translations.

This thesis investigates band topologies which rely fundamentally on spatial symmetries. The first part of the thesis addresses topological phases with discretely-robust surface properties – I offer two case studies in this regard, one symmmorphic and the other nonsymmmorphic. How are surface modes robust? I propose a sufficient criterion on the protective symmetry group. Minimally, (i) the symmetry must be unbroken by the presence of the surface. Additionally, either (ii) a reflection symmetry exists so that mirror-subspaces can display a quantum anomalous Hall effect, or (iii) there exist at least two high-symmetry points in the surface Brillouin zone (BZ), which admit higher-than-one dimensional irreducible representations (irreps) of the symmetry group. In addition to predicting new topological materials, these criteria are also satisfied by the well-known SnTe class, [7] and also the $\mathbb{Z}_2$ insulators. [3, 8–17] Among the 32 crystallographic point groups, only the $C_n$ and $C_{nv}$ groups are preserved for a surface that is orthogonal to the rotational axis. [18] Though all $C_{nv}$ groups satisfy (ii), the lack of spin-orbit coupling implies only $C_{3v}$ systems can have nonvanishing mirror Chern numbers. While all $C_n$ groups by themselves only have one-dimensional irreps, the $C_4$ or $C_6$ group satisfies (iii) in combination with TRS, as is known for the topological crystalline insulators introduced in Ref. [19]. Finally, only $n = 3, 4$ and 6 of the $C_{nv}$ groups possess two-dimensional irreps which satisfy (iii). In Chapter 3, I describe the first-known 3D topological insulators without spin-orbit coupling, and with surface modes that are protected only by point groups ($C_{3v}$, $C_{4v}$ and $C_{6v}$), i.e., the relevant symmetries are purely crystalline and do not include time-reversal. To describe these $C_{nv}$ systems, I introduce the notions of (a) a halved-mirror chirality: an integer invariant which characterizes half-mirror planes in the 3D Brillouin zone, and (b) a bent Chern number: the
traditional TKNN invariant generalized to bent 2D manifolds.

To motivate how non-symmorphic space groups result in robust surface properties, we add a fourth criterion that generalizes (iii) in a nontrivial way: (iv) there exists two separated, high-symmetry submanifolds in the surface BZ, which admit higher-than-one dimensional elementary band representations. Elementary band representations are band representations which cannot be decomposed as direct sums, [20] and there are enough contact points to continuously travel through all its branches; this property of ‘connectivity’ is a well-known feature of non-symmorphic space groups. [21] A precise statement of this symmetry criterion (in Part IV) applies to all known symmetry-protected surface topologies. For now, we particularize to a specific example: for spin systems with glide-reflection and time-reversal symmetries, the elementary band representation is four-dimensional and looks like the cross-section of an hourglass. Hourglasses can be found on two, separated glide-invariant lines in the surface BZ – in the intervening space, it is possible for surface bands to connect one hourglass to the next in an unbreakable zigzag pattern. In Chapter 4, I propose that this hourglass-zigzag connectivity is found in the large-gap insulators: KHgX (X = As, Sb and Bi), which is the first material class whose topology relies on non-symmorphic symmetries.

The hourglass-zigzag connectivity is an example of a sub-topology, in the sense that it describes only a submanifold of the BZ. There are other sub-topologies which are realizable in the same nonsymmmorphic group; they include: a glide-symmetric analog of the quantum spin Hall effect (as realized by Dirac-semimetallic Na$_3$Bi under pressure) and quantized non-Abelian polarizations. The various sub-topologies must be pieced together to form a globally consistent topology – in this sense our insulators are ‘piecewise topological’. In Chapter 5, I propose an efficient method to piece together sub-topologies through the Wilson loop, which represents parallel transport in quasimomentum space. Our methodology necessitates the extension of the ordinary crystal group by Wilson loops – such an ex-
tended group describes generalized symmetries that combine space-time transformations with quasimomentum translations; the different extensions are classified by group cohomology. Our finding generalizes the construction of non-symmorphic space groups, which extends point group by real-space translations. Here, we further extend non-symmorphic groups by reciprocal translations, thus placing real and quasimomentum space on equal footing. A consequence of this projective representation is an atypical bulk-boundary correspondence for our topological insulators.

The second part of the thesis addresses topological phases without surface properties – their only known physical consequences are discrete signatures in parallel transport. We provide two such case studies with spatial-inversion and discrete-rotational symmetries respectively. One lesson learned here regards the choice of parameter loops in which we carry out transport – the loop must be chosen to exploit the symmetry that protects the topology. Straight loops are a natural choice with spatial inversion symmetry, since such a loop can be mapped to itself up to a change of orientation. My straight analysis in Chapter 6 shows that centrosymmetric insulators have a $\mathbb{Z} \geq$ classification in one and two spatial dimensions. The 2D invariant describes a $\mathbb{Z} \geq$ relative winding of the non-Abelian Berry phases, which are obtained from the eigenspectrum of the Wilson loop. In comparison, the first Chern class describes a center-of-mass winding, while the quantum spin Hall phase manifests a $\mathbb{Z}_2$ relative winding.

While straight loops are popular for their connection with the geometric theory of polarization, Chapter 7 describes the first application of bent loops in topological band theory. One bends the loop such that half the loop is mapped to the other half by discrete rotations – this leads to quantized non-Abelian Berry phases in the presence of rotational ($C_4$ and $C_6$) and time-reversal symmetries. Time-reversal symmetry plays an important role in making the Wilson loops essentially real, which leads to a connection with the theory of matrices in $SO(2m)$ – different sectors of gapped groundstates have a one-to-one correspondence with
distinct classes of equiangular rotations.
Part II

Preliminaries

The first two chapters pedagogically introduce the tight-binding method (in Chap. 1) and Brillouin-zone Wilson loops (in Chap. 2). The experienced reader may jump on to the Thesis body in Part III, and refer back when necessary.
Chapter 1

Symmetries of tight-binding Hamiltonians

After introducing the tight-binding method in Sec. 1.1, we consider the effect of spatial symmetries in Sec. 1.2, then generalize our discussion to space-time symmetries in Sec. 1.3. The useful notion of a little group is introduced in Sec. 1.4 and 1.5.

1.1 Review of the tight-binding Hamiltonian

In the tight-binding variational approximation, the Hilbert space is reduced to $n_{\text{tot}}$ atomic orbitals $\phi_\alpha(r - R - r^{(\alpha)})$; $\phi_\alpha$ are eigenstates of an atomic Hamiltonian, and $\alpha = 1, 2, \ldots, n_{\text{tot}}$ denotes orbital and spin. $R$ is a Bravais lattice vector that denotes a unit cell. Within each unit cell, $r^{(\alpha)}$ is the position of the atom corresponding to orbital $\alpha$. Due to the finite overlap of atomic orbitals, we are motivated to construct an orthonormal basis that preserves the point-group symmetries of $\phi_\alpha$. Such a basis is realized with Löwdin functions, [22–24] which are defined as

$$
\varphi_\alpha(x - R_i - r^{(\alpha)}) = \sum_{j, \beta} \phi_\beta(x - R_j - r^{(\beta)}) \left[ \Delta^{-1/2} \right]_{ji}^{\beta \alpha}
$$

(1.1)
with the hermitian overlap integral

$$\Delta_{ij}^{\alpha \beta} = \int d^3r \phi_\alpha^*(x - R_i - r^{(\alpha)}) \phi_\beta(x - R_j - r^{(\beta)}). \quad (1.2)$$

Here, $i,j$ are indices for Bravais lattice (BL) vectors; we sum over repeated indices. The orthogonality of Löwdin function reads as

$$\int d^3r \varphi_\alpha^*(x - R_i - r^{(\alpha)}) \varphi_\beta(x - R_j - r^{(\beta)}) = \delta_{\alpha \beta} \delta_{i,j}. \quad (1.3)$$

In Hamiltonians with discrete translational symmetry, our basis vectors are

$$\phi_{k,\alpha}(r) = \frac{1}{\sqrt{N}} \sum_R e^{i\mathbf{k} \cdot (\mathbf{R} + \mathbf{r}_\alpha)} \varphi_{\mathbf{R},\alpha}(r - \mathbf{R} - \mathbf{r}_\alpha), \quad (1.4)$$

which are periodic in lattice translations $\mathbf{R}$. $\mathbf{k}$ is a crystal momentum, $N$ is the number of unit cells, $\alpha$ labels the Löwdin orbital, and $\mathbf{r}_\alpha$ denotes the position of the orbital $\alpha$ as measured from the origin in each unit cell. The tight-binding Hamiltonian is defined as

$$H(\mathbf{k})_{\alpha \beta} = \int d^3r \phi_{k,\alpha}(r)^* \hat{H} \phi_{k,\beta}(r), \quad (1.5)$$

where $\hat{H}$ is the single-particle Hamiltonian. The energy eigenstates are labelled by a band index $n$, and defined as $\psi_{n,k}(r) = \sum_\alpha u_{n,k}(\alpha) \phi_{k,\alpha}(r)$, where

$$\sum_\beta H(\mathbf{k})_{\alpha \beta} u_{n,k}(\beta) = \varepsilon_{n,k} u_{n,k}(\alpha). \quad (1.6)$$

We employ the braket notation:

$$H(\mathbf{k}) | u_{n,k} \rangle = \varepsilon_{n,k} | u_{n,k} \rangle. \quad (1.7)$$

Due to the spatial embedding of the orbitals, the basis vectors $\phi_{k,\alpha}$ are generally not periodic under $\mathbf{k} \to \mathbf{k} + \mathbf{G}$ for a reciprocal lattice (RL) vector $\mathbf{G}$. This implies that the tight-binding Hamiltonian satisfies:

$$H(\mathbf{k} + \mathbf{G}) = V(\mathbf{G})^{-1} H(\mathbf{k}) V(\mathbf{G}), \quad (1.8)$$

where $V(\mathbf{G})$ is a unitary matrix with elements: $[V(\mathbf{G})]_{\alpha \beta} = \delta_{\alpha \beta} e^{i\mathbf{G} \cdot \mathbf{r}_\alpha}$. 
This thesis describes Hamiltonians each with a spectral gap that is finite for all $k$, such that we can distinguish occupied from empty bands. Let $P$ project to the occupied bands as

$$P = \sum_{k \in BZ} P(k) \quad \text{and} \quad P(k) = \sum_{n=1}^{n_{\text{occ}}} |u_{n,k}\rangle\langle u_{n,k}| = V(G) P(k + G) V(G)^{-1}. \quad (1.9)$$

### 1.2 Effect of spatial symmetries on the tight-binding Hamiltonian

Let us denote a spatial transformation by $g_\delta$, which transforms real-space coordinates as $r \rightarrow D_g r + \delta$, where $D_g$ is the orthogonal matrix representation of the point-group transformation $g$ in $\mathbb{R}^d$. Non-symmorphic space groups contain symmetry elements where $\delta$ is a rational fraction [6] of the lattice period; in a symmorphic space group, an origin can be found where $\delta = 0$ for all elements. The purpose of this Section is to derive the constraints of $g_\delta$ on the tight-binding Hamiltonian. First, we clarify how $g_\delta$ transforms the creation and annihilation operators. We define the creation operator for a L"{o}wdin function $\varphi_{R,\alpha}$ as $c^\dagger_{\alpha}(R + r_\alpha)$. From (1.4), the creation operator for a Bloch basis vector $\phi_{k,\alpha}$ is

$$c^\dagger_{k,\alpha} = \frac{1}{\sqrt{N}} \sum_R e^{ik \cdot (R + r_\alpha)} c^\dagger_{\alpha}(R + r_\alpha). \quad (1.10)$$

Let $U_{g_\delta}$ be the unitary representation of $g_\delta$ in the basis of L"{o}wdin orbitals. The creation operator transforms as

$$g_\delta : c^\dagger_{\alpha}(R + r_\alpha) \rightarrow c^\dagger_{\beta}(D_g R + R_{\beta \alpha}^{\delta} + r_\beta) [U_{g_\delta}]_{\beta \alpha}. \quad (1.11)$$

Here, we have defined $R_{\beta \alpha}^{\delta} = D_g r_\alpha + \delta - r_\beta$. A Bravais lattice (BL) that is symmetric under $g_\delta$ satisfies two conditions:

(i) for any BL vector $R$, $D_g R$ is also a BL vector:

$$\forall R \in \text{BL}, \quad D_g R \in \text{BL}. \quad (1.12)$$
(ii) If \( g \) transforms an orbital of type \( \alpha \) to another of type \( \beta \), i.e., \( [U_{g\delta}]_{\beta\alpha} \) is nonzero, then \( D_g(R + r_\alpha) + \delta \) must be the spatial coordinate of an orbital of type \( \beta \):

\[
[U_{g\delta}]_{\beta\alpha} \neq 0 \Rightarrow R_{\beta\alpha}^{g\delta} \in \text{BL}. \tag{1.13}
\]

For fixed \( g, \alpha \) and \( \beta \), the mapping \( T_{\beta\alpha}^{g\delta} : R \rightarrow R_{\beta\alpha}^{g\delta} \) is bijective. Applying (1.10), (1.12), (1.13), the orthogonality of \( D_g \) and the bijectivity of \( T_{\beta\alpha}^{g\delta} \), the Bloch basis vectors transform as

\[
g_{\delta} : c^\dagger_{k,\alpha} \rightarrow e^{-i(D_gk)\delta}c^\dagger_{D_gk,\beta}[U_{g\delta}]_{\beta\alpha}. \tag{1.14}
\]

This motivates a definition of the operator

\[
\hat{g}_{\delta}(k) \equiv e^{-i(D_gk)\delta}U_{g\delta}, \tag{1.15}
\]

which acts on Bloch wavefunctions \((|u_{n,k}⟩)\) as

\[
g_{\delta} : |u_{n,k}⟩ \rightarrow \hat{g}_{\delta}(k)|u_{n,k}⟩. \tag{1.16}
\]

The operators \( \{\hat{g}_{\delta}(k)\} \) represent the space-group algebra [6] in a basis of Bloch waves. If the space group is non-symmorphic, the nontrivial phase factor \( \exp(-i(D_gk) \cdot \delta) \) in \( \hat{g}_{\delta}(k) \) encodes the effect of the fractional translation, i.e., the momentum-independent matrices \( \{U_{g\delta}\} \) by themselves form a representation of a point group.

To exemplify this abstract discussion, we analyze a simple 2D non-symmorphic crystal in Fig. 1.1(a), which may be interpreted as the Hg atoms in the top atomic layer of the 010 surface of KHgSb. As delineated by a square, the unit cell comprises two atoms labeled by subcell coordinates \( A \) (dark blue) and \( B \) (cyan), and the spatial origin is chosen at their midpoint, such that \( r_A = a\bar{x}/\sqrt{3} - cz/2 = -r_B \). The symmetry group \((Pma2)\) of this lattice is generated by the elements \( M_{z,c\bar{x}/2} \) and \( M_{z,c\bar{x}/2} \), where in the former we first reflect across \( \bar{x} \) (as illustrated in Fig. 1.1(b) \( \rightarrow \) (c)) and then translate by \( \delta = c\bar{z}/2 \) (Fig. 1.1(c) \( \rightarrow \) (d)). Let us represent these symmetries with spin-doubled \( s \) orbitals on each atom. Choosing our
Figure 1.1: (a) Simple example of a 2D non-symmorphic crystal. The two sublattices are colored respectively colored dark blue and cyan. (b-d) illustrate the effect of a glide reflection.

basis to diagonalize the spin component ($S_z$) along $\vec{z}$,

$$
M_{x,c\vec{z}/2} : \begin{cases} 
    c_{A,S_z}^\dagger (\vec{R} + \vec{r}_A) &\rightarrow -ic_{B,-S_z}^\dagger (D_x\vec{R} + \vec{r}_B), \\
    c_{B,S_z}^\dagger (\vec{R} + \vec{r}_B) &\rightarrow -ic_{A,-S_z}^\dagger (D_x\vec{R} + c\vec{z} + \vec{r}_A),
\end{cases}
$$

where $D_x(x,z)^t = (-x,z)^t$. It is useful to recall here that a reflection is the product of an inversion with a two-fold rotation about the reflection axis: $M_j = IC_{2j}$ for $j \in \{x,z\}$. Consequently, $M_{x,c\vec{z}/2} \propto C_{2x}$ flips $S_z \rightarrow -S_z$. In the basis of Bloch waves,

$$
M_{x,c\vec{z}/2} : c_{k,\alpha}^\dagger \rightarrow e^{-ik_{x}c/2}c_{D_xk,\beta}^\dagger [U_{x,c\vec{z}/2}]_{\beta\alpha} \quad \text{with} \quad U_{x,c\vec{z}/2} = -i\tau_3 \sigma_1.
$$

Here, we have employed $\tau_3 = +1 (-1)$ for subcell $A (B)$ and $\sigma_3 = +1$ for spin up. A similar
analysis for the other reflection leads to

\[
M_{z,c\hat{z}/2} : \begin{cases} 
    c_{A,Sz}^\dagger (R + r_A) \rightarrow -i \text{sign}[S_z] c_{A,Sz}^\dagger (D_z R + c\hat{z} + r_A), \\
    c_{B,Sz}^\dagger (R + r_B) \rightarrow -i \text{sign}[S_z] c_{B,Sz}^\dagger (D_z R + r_B),
\end{cases}
\]  \hspace{1cm} (1.19)

with \(D_z(x,z) = (x,-z)^t\), and in the Bloch-wave basis,

\[
M_{z,c\hat{z}/2} : c_{k,\alpha}^\dagger \rightarrow e^{-ik_z c/2} c_{D_z k,\beta}^\dagger [U_{z,c\hat{z}/2}]_{\beta\alpha} \quad \text{with} \quad U_{z,c\hat{z}/2} = -i \sigma_3.
\]  \hspace{1cm} (1.20)

To recapitulate, we have derived \(\{\hat{g}_\delta\}\) as

\[
\hat{M}_{x,c\hat{z}/2}(k) = -ie^{-ik_z c/2} \tau_1 \sigma_1 \quad \text{and} \quad \hat{M}_{z,c\hat{z}/2}(k) = -ie^{-ik_z c/2} \sigma_3,
\]  \hspace{1cm} (1.21)

which should satisfy the space-group algebra for \(Pma2\), namely that

\[
M_{x,c\hat{z}/2}^2 = \bar{E} t(c\hat{z}) , \quad M_{z,c\hat{z}/2}^2 = \bar{E} , \quad \text{and} \quad M_{x,c\hat{z}/2} M_{x,c\hat{z}/2} = \bar{E} t(-c\hat{z}) M_{x,c\hat{z}/2} M_{x,c\hat{z}/2},
\]  \hspace{1cm} (1.22)

where \(\bar{E}\) denotes a \(2\pi\) rotation and \(t(c\hat{z})\) a translation. Indeed,

\[
\hat{M}_{x,c\hat{z}/2}(D_z k) \hat{M}_{x,c\hat{z}/2}(k) = -e^{-ik_z c}, \quad \hat{M}_{z,c\hat{z}/2}(D_z k) \hat{M}_{z,c\hat{z}/2}(k) = -I, \quad \text{and} \quad \hat{M}_{x,c\hat{z}/2}(D_z k) \hat{M}_{z,c\hat{z}/2}(k) = -e^{-ik_z c} \hat{M}_{x,c\hat{z}/2}(D_z k) \hat{M}_{z,c\hat{z}/2}(k).
\]  \hspace{1cm} (1.23)

Finally, we verify that the momentum-independent matrices \(\{U_{g\delta}\}\) form a representation of the double point group \(C_{2v}\), whose algebra is simply

\[
M_x^2 = M_z^2 = \bar{E} \quad \text{and} \quad M_z M_x = \bar{E} M_x M_z.
\]  \hspace{1cm} (1.24)

A simple exercise leads to

\[
U_{x,c\hat{z}/2}^2 = U_{x,c\hat{z}/2}^2 = -I \quad \text{and} \quad \{U_{x,c\hat{z}/2},U_{x,c\hat{z}/2}\} = 0.
\]  \hspace{1cm} (1.25)

The algebras of \(C_{2v}\) and \(Pma2\) differ only in the additional elements \(t(\pm c\hat{z})\), which in the Bloch-wave representation (\(\{\hat{g}_\delta(k)\}\)) is accounted for by the phase factors \(\exp(-ik_z c/2)\).
Returning to a general discussion, if the Hamiltonian is symmetric under $g_\delta$, Eq. (1.14) implies

\[
\hat{g}_\delta(k) \, H(k) \, \hat{g}_\delta(k)^{-1} = H(Dg \, k).
\]

(1.26)

By assumption of the insulating gap, $\hat{g}_\delta(k)|u_{n,k}\rangle$ belongs in the occupied-band subspace for any occupied band $|u_{n,k}\rangle$. This implies a unitary matrix representation of $g_\delta$ in the occupied-band subspace:

\[
[\tilde{g}_\delta(Dg \, k + G, k)]_{mn} = \langle u_{m,Dg \, k+G} | V(-G) \, \hat{g}_\delta(k) | u_{n,k}\rangle, \quad \text{with} \quad m, n = 1, \ldots, n_{\text{occ}},
\]

(1.27)

and $G = k - Dg \, k$ is any reciprocal vector (including zero). We will often use the shorthand: $\hat{g}_\delta(k) \equiv \tilde{g}_\delta(Dg \, k, k)$, since the second argument is self-evident. We emphasize that $\hat{g}_\delta$ and $\tilde{g}_\delta$ are different matrix representations of the same symmetry element ($g_\delta$), and moreover the matrix dimensions differ: (i) $\hat{g}_\delta$ acts on Bloch-combinations of Löwdin orbitals ($\{\phi_{k,\alpha} | \alpha = 1, \ldots, n_{\text{tot}}\}$) defined in Eq. (1.4), while (ii) $\tilde{g}_\delta$ acts on the occupied eigenfunctions ($\{u_{n,k} | n = 1, \ldots, n_{\text{occ}}\}$) of $H(k)$. It will often be convenient to move freely between the two representations. It will also be useful to understand the commutative relation between $\hat{g}_\delta(k)$ and the diagonal matrix $V(G)$ defined in Eq. (1.8). From Eq. (1.12) and (1.13),

\[
[U_{g \delta}]_{\alpha\beta} \neq 0 \quad \Rightarrow \quad Dg^{-1}R_{\alpha\beta}^{\delta} \in \text{BL} \quad \Rightarrow \quad e^{iG \cdot (r_{\alpha} + Dg^{-1}d - Dg^{-1}r_{\alpha})} = 1,
\]

(1.28)

for a RL vector $G$. We then derive

\[
\hat{g}_\delta(k) \, V(G) = e^{-iDg \, G \cdot \delta} \, V(Dg \, G) \, \hat{g}_\delta(k).
\]

(1.29)

This equality applies only if the argument of $V$ is a RL vector.
1.3 Effect of space-time symmetry on the tight-binding Hamiltonian

Consider a general space-time transformation $T g_δ$, where now we include the time-reversal $T$; the following discussion also applies if $g_δ$ is the trivial transformation.

$$T g_δ : c_α^+(R + r_α) \rightarrow c_β^+(D g_R + R_{βα}^T g + r_β) \left[ U_{T g_δ} \right]_{βα},$$

(1.30)

where $U_{T g_δ}$ is the matrix representation of $T g_δ$ in the orbital basis, $R_{βα}^T g = D g r_α + δ - r_β$,

$$[U_{T g_δ}]_{βα} \neq 0 \Rightarrow R_{βα}^T g \in \text{BL},$$

(1.31)

and the Bravais-lattice mapping of $R$ to $D g R + R_{βα}^T g$ is bijective. It follows that the Bloch waves transform as

$$T g_δ : c_{k,α}^+ \rightarrow e^{i D g k \cdot δ} c_{−D g k,β}^+ \left[ U_{T g_δ} \right]_{βα}.$$ 

(1.32)

This motivates the definition of the operator

$$\hat{T}_{g_δ}(k) \equiv e^{i(D g k \cdot δ)} U_{T g_δ} K,$$

(1.33)

which implies of a $T g_δ$-symmetric Hamiltonian:

$$\hat{T}_{g_δ}(k) H(k) \hat{T}_{g_δ}(k)^{-1} = H(−D g k).$$

(1.34)

For a simple illustration, we return to the lattice of Fig. 1.1, where time-reversal symmetry is represented by $\hat{T}(k) = −iσ_2 K$, which commutes with any spatial transformation:

for $j \in \{x, z\}$, \( \hat{T}(D_j k) \hat{M}_{j,ε/2}(k) = \hat{M}_{j,ε/2}(−k) \hat{T}(k). \)

(1.35)

If the Hamiltonian is gapped, there exists an antiunitary representation of $T g_δ$ in the occupied-band subspace:

$$[\hat{T}_{g_δ}(G − D_g k, k)]_{mn} = \langle u_{m, G − D_g k} | V(−G) \hat{T}_{g_δ}(k) | u_{n, k} \rangle, \quad \text{with} \quad m, n = 1, \ldots, n_{\text{occ}}.$$

(1.36)
Once again, we introduce the shorthand: $\hat{T}_g(k) \equiv \hat{T}_g(-D_g k, k)$. Eq. (1.31) and (1.12) further imply that

$$[U_T]_{\alpha\beta} \neq 0 \Rightarrow D_g^{-1} R_{\alpha\beta} \in \text{BL} \Rightarrow e^{i G \cdot (r_\beta + D_g^{-1} \delta - D_g^{-1} r_\alpha)} = 1,$$

(1.37)

finally leading to

$$\hat{T}_g(k) V(G) = e^{i D_g G \cdot \delta} V(-D_g G) \hat{T}_g(k).$$

(1.38)

### 1.4 Little group of the wavevector

Suppose special momenta $(\bar{k})$ exist that satisfies

$$D(g) \bar{k} = \bar{k} + G_g(\bar{k})$$

(1.39)

for some reciprocal lattice (RL) vector $G$ that depends on the momentum and the symmetry element in question. We say that $\bar{k}$ as invariant under $g$. We deduce from (1.8) that

$$[H(\bar{k}), V(G_g(\bar{k})) U(g)] = 0.$$

(1.40)

Equivalently, the eigenstates of $H(\bar{k})$ may be chosen to have quantum numbers under the unitary operation $V(G_g(\bar{k})) U(g)$. The collection of all symmetry elements $\{g_1, g_2, \ldots, g_l\}$ which leave $\bar{k}$ invariant forms the little group of the wavevector; the little group is generically a subgroup of the group of the Hamiltonian. [18] Henceforth, we shall be discussing a single momentum $\bar{k}$, and we suppress writing $\bar{k}$ in the arguments of $G_g$. The set of operations $\{V(G_{g_1}) U(g_1), \ldots, V(G_{g_l}) U(g_l(\bar{k}))\}$ form a representation of the little group at $\bar{k}$. The little group at $\bar{k} = 0$ is the group of the Hamiltonian, for which $\{U(g_1), \ldots, U(g_l(0))\}$ form a representation; in this case $V(G_g) = I$ trivially for all $g$.

Let’s introduce the shorthand: $D_a = D(g_a)$ and $U(g_a) = U_a$. A useful identity is

$$U_a V(G) U^{-1}_a = V(D_a G)$$

(1.41)

for any reciprocal lattice vector $G$. Proof: applying (1.12) and (1.13), we deduce that

$$[U_a]_{\alpha\beta} \neq 0 \Rightarrow D_a^{-1} \Delta_{\alpha\beta} \in \text{BL}.$$

(1.42)
Applying this in conjunction with the orthogonality of $D_a$, we find

$$[U_a V(G)]_{\alpha\beta} = [U_a]_{\alpha\beta} e^{iG \cdot r_\beta} = e^{i(D_a G) \cdot r_\alpha} [U_a]_{\alpha\beta} e^{iG D_a^{-1} \Delta_{\alpha\beta}} = [V(D_a G) U_a]_{\alpha\beta}. \quad (1.43)$$

For a less trivial example of a little group, we consider the $C_4$-invariant point $\bar{k} = (\pi, \pi, 0)$ for spinless $C4v$ systems. Each element $g_a$ in this group is represented by $X(g_a) = V(G_{g_a}) U(g_a)$:

$$X(e) = I, \quad X(C_4) = V(-2\pi \hat{x}) U(C_4),$$
$$X(C_2) = V(-2\pi(\hat{x} + \hat{y})) U(C_2), \quad X(M_x) = V(-2\pi \hat{x}) U(M_x),$$
$$X(M_1) = U(M_1), \quad X(M_2) = V(-2\pi(\hat{x} + \hat{y})) U(M_2),$$
$$X(C_4^{-1}) = V(-2\pi \hat{y}) U(C_4^{-1}), \quad X(M_y) = V(-2\pi \hat{y}) U(M_y), \quad (1.44)$$

where $e$ is the identity element, $C_n$ is an $n$-fold rotation, and $M_i$ are reflections which transform real-space coordinates as $M_x : (x, y) \rightarrow (-x, y)$, $M_y : (x, y) \rightarrow (x, -y)$, $M_1 : (x, y) \rightarrow (y, x)$, $M_2 : (x, y) \rightarrow (-y, -x)$. Applying (1.41), one derives that these matrices satisfy the requisite algebraic relations, e.g., $X(C_4)^4 = X(e)$, $X(M_i)^2 = X(e)$ and $X(M_i) X(C_4) X(M_i)^{-1} = X(C_4^{-1})$. The last relation is merely the matrix representation of a simple statement: the handedness of a rotation inverts under a reflection, if the rotation axis is parallel to the reflection plane.

### 1.5 Generalized little groups

Let us consider lower-dimensional submanifolds which are embedded in the 3D BZ. The set of all elements which leave this submanifold invariant is defined as the little group of the submanifold. The little group of the wavevector corresponds to a 0D submanifold, but we will also be interested in 1D and 2D submanifolds. For example, let us define a mirror plane (MP) as a plane in the 3D BZ which is mapped to itself under a certain reflection, up to a translation by a RL vector. For example, the plane $k_x = \pi$ is mapped to itself under the reflection $M_x : (x, y) \rightarrow (-x, y)$, up to a translation of $G = 2\pi \hat{x}$. We define the group of the MP as the collection of all symmetry elements $\{g_1, g_2, \ldots, g_l\}$ which leave MP invariant;
the group of the MP is generically a subgroup of the group of the Hamiltonian, which we take to be $C_{4v}$ for illustration. In the spinless representation, the group of the MP $k_x = \pi$ consists of the elements \{e, $M_x$, $C_2$, $M_y$\}. We recall the definitions of $U(g)$, $D(g)$ and $V(k)$ in Sec. 1.2. Suppose $k \in MP$, $G_g(MP)$ is defined as the RL vector that separates $D(g)k$ from the MP:

$$\forall \, k, k' \in MP, \quad D(g)k = k' + G_g(MP). \quad \text{(1.45)}$$

Each element in the group of the MP is represented by $X(g) = V(G_g(MP))U(g)$. For example, the group of the MP $k_x = \pi$ is represented by

$$
\begin{align*}
X(e) &= I, & X(C_2) &= V(-2\pi \hat{x})U(C_2), \\
X(M_x) &= V(-2\pi \hat{x})U(M_x), & X(M_y) &= U(M_y). \quad \text{(1.46)}
\end{align*}
$$

One may verify through the identity (1.41) that these matrices satisfy the requisite algebraic relations, e.g., $X(C_2)^2 = X(e)$, and $X(M_x)X(C_2)X(M_x^{-1}) = X(C_2^{-1}) = X(C_2)$. 


Chapter 2

Introduction to Brillouin-zone Wilson loops

In search for a tool to identify topological structure in bands, we note that the description of translationally-invariant insulators has a local gauge redundancy – its ground state is invariant under a unitary transformation in the subspace of occupied bands. Since all topological quantities must be invariant under this transformation, the natural objects to investigate are the Berry phase factors acquired around a loop, which are known to be gauge-invariant quantities. We are proposing that distinct bands can be distinguished by holonomy, i.e., parallel transport through certain non-contractible loops in the Brillouin zone. Holonomies are known to have diverse applications in physics. [25] The matrix representation of parallel transport is called a Wilson loop ($W$), and its eigenspectrum comprise the non-Abelian Berry phase factors. [26–29]

This Chapter is a pedagogical introduction to Brillouin-zone Wilson loops; we describe its role in holonomy (Sec. 2.1) and in the geometric-phase theory of polarization (Sec. 2.2). In Sec. 2.3, we explain the construction of a coarse-grained Wilson loop from a tight-binding Hamiltonian, for the purpose of numerically computing topological invariants. Basic analytic properties are described in Sec. 2.4.
The Hamiltonian for a single particle is

\[ H = \frac{p^2}{2m} + V(r). \]  \hspace{1cm} (2.1)

If \( V(r) = V(r + R) \) for any lattice vector \( R \), this Hamiltonian is symmetric under discrete translations. Consequently, \( H \) decouples into representations labelled by the crystal momentum \( k \); an eigenstate in the \( n' \)th band may be written in Bloch form: \( \psi_{kn}(r) = e^{ikr} u_{kn}(r) \), where \( u_{kn}(r) = u_{kn}(r + R) \) is a function that is periodic in lattice translations, and also satisfies:

\[ \left[ \frac{(p + \hbar k)^2}{2m} + V(r) - \varepsilon_{kn} \right] u_{kn}(r) = 0. \]  \hspace{1cm} (2.2)

Each eigenstate has a corresponding projection \( P_{kn}(r, r') = u_{kn}(r) u_{kn}^\ast(r') \); the many-body ground-state is a single Slater determinant of all single-particle eigenstates with energies less than the Fermi energy. The topological properties of an insulator are invariant under transformations of the Hamiltonian that preserve both the energy gap and the symmetry that stabilizes the topological phase. We perform one such transformation by setting the energies of all eigenstates \( u_{kn} \) below (above) the Fermi energy equal to \( \varepsilon_- (\varepsilon_+) \). Denoting the projection onto the \( n_{\text{occ}} \) occupied bands as \( P_{k}^{\text{occ}} = \sum_{i=1}^{n_{\text{occ}}} P_{kn} \), we express the resultant flat-band Hamiltonian as

\[ \mathcal{H}_F(k) = (\varepsilon_- - \varepsilon_+) P_{k}^{\text{occ}} + \varepsilon_+ I. \]  \hspace{1cm} (2.3)

Eq. (2.3) has a gauge redundancy which is not apparent in (2.2) – the ground-state projection \( P_{k}^{\text{occ}} \) is invariant under a local \( U(n_{\text{occ}}) \) gauge transformation in the \( n_{\text{occ}} \)-dimensional subspace of occupied bands: \( u_{kn} \rightarrow u_{km} M_{kn}^{\text{occ}} \) with \( m, n = 1 \ldots n_{\text{occ}} \) and \( M_{kn}^1 = M_{kn}^\dagger \).

### 2.1 Wilson Loop as arising from Holonomy

The adiabatic transport of a ground state at initial momentum \( k^{(i)} \) to a final momentum \( k \) involves a unitary rotation of the basis vectors \( u_{kn} \) in the subspace of occupied bands.
This $U(n_{\text{occ}})$ rotation is affected by a Wilson-line matrix $W_{k \rightarrow k(i)}$ that maps the subspace of occupied bands at $k^{(i)}$ to the subspace of occupied bands at $k$. $W$ is known to satisfy a parallel transport equation

$$\frac{\partial}{\partial k_{\mu}} W_{k \rightarrow k(i)} = -C_{\mu}(k) W_{k \rightarrow k(i)}, \quad (2.4)$$

with the Berry-Wilczek-Zee connection $C$ defined as [26, 27]

$$C_{\mu \nu}^{mn}(k) = \int d^d r \ u_m^*(k(r)) \frac{\partial}{\partial k_{\mu}} u_n(k(r)). \quad (2.5)$$

Here, $k_{\mu} \in \{k_1, \ldots, k_d\}$ denote momenta components in a $d$-dimensional BZ. We proceed to derive Eq. (2.4). Upon adiabatic evolution through the Brillouin zone, the state $u_{k(i)}^n$ at some initial momentum $k(i)$ (at time $t_i$) is mapped to a different state $v_k^n$ at final momentum $k$ (at time $t$). In this process, the state acquires a dynamical phase $\int_{t_i}^t \varepsilon \, dt$. In addition, there is a unitary rotation of basis vectors in the occupied subspace; this rotation is affected by a $U(n_{\text{occ}})$ Wilson-line matrix $W_{k \rightarrow k(i)}$:

$$v_k^n(r) = e^{-i \int_{t_i}^t \varepsilon \, dt} \sum_{m=1}^{n_{\text{occ}}} u_{k(i)}^m(r) W_{k \rightarrow k(i)}^{mn}. \quad (2.6)$$

Let us apply the time-dependent Schrödinger equation:

$$\mathcal{H}_t(k) v_k^n(r) = i \partial_t \left[ e^{-i \int_{t_i}^t \varepsilon \, dt} \sum_m u_{k(i)}^m(r) W_{k \rightarrow k(i)}^{mn} \right]. \quad (2.7)$$

In the adiabatic approximation, $v_k^n$ remains an eigenstate of the $\mathcal{H}_k(k)$ with energy $\varepsilon$. Upon cancellation of the dynamical phase and replacing $\partial_t = \sum_{\mu=1}^d (dk_{\mu}/dt) \partial_{k_{\mu}}$ for a $d$-dimensional BZ, we arrive at Eq. (2.4).

This differential equation has the path-ordered solution

$$W_{k \rightarrow k(i)}(\mathcal{L}) = T \exp \left[ - \int_{\mathcal{L}} C_{\mu}(q) \, dq_{\mu} \right] \quad (2.8)$$

for a path $\mathcal{L}$ that connects momenta $k$ and $k(i)$. If $k = k(i)$ modulo a reciprocal lattice vector, $\mathcal{L}$ forms a non-contractible loop in the BZ; we denote the resultant $U(n_{\text{occ}})$ Wilson loop as $\mathcal{W}$:

$$\mathcal{W} = T \exp \left[ - \int dk_{\mu} C_{\mu}(k) \right]. \quad (2.9)$$
As Zak demonstrated for \( n_{\text{occ}} = 1 \), the Abelian \( W \) is nothing less than the Berry phase factor acquired by a Bloch wave around a cyclic evolution. [29] For general \( n_{\text{occ}} \), (2.9) forms a matrix representation of a holonomy, \( i.e., \) a parallel transport map. [25] The eigenvalues of this matrix are the non-Abelian Berry phase factors, which quantify a change relative to a periodic gauge, defined as \( \psi^m_k = \psi^m_{k+2\pi} \); the phase factors are invariant under gauge transformations that preserve this periodic condition.

### 2.2 Wilson Loops in the Geometric-Phase Theory of Polarization

Let us derive a well-known relation between \( W \) and the polarization of a 1D insulator. For a group of \( n_{\text{occ}} \) occupied bands, the delocalized Bloch waves \( \psi^m_k \) form an orthonormal basis in the occupied Hilbert space; \( m = 1, 2, \ldots, n_{\text{occ}} \). Assuming a periodic gauge (\( \psi^m_k = \psi^m_{k+2\pi} \)), we formulate the theory of polarization in an alternative basis of localized Wannier functions (WF):

\[
\Psi^{(j)}(x - R) = \int \frac{dk}{2\pi} e^{-ikR} \sum_{n=1}^{n_{\text{occ}}} O(k)_{jn} \psi^n_k(x).
\]  

(2.10)

Each WF \( \Psi^{(j)}(x - R) \) is labelled by the unit cell \( R \in \mathbb{Z} \) and an index \( j = 1, 2, \ldots, n_{\text{occ}} \). If \( n_{\text{occ}} = 1 \), \( O(k) \) is a momentum-dependent phase; if \( n_{\text{occ}} > 1 \), \( O(k) \) is a \( U(n_{\text{occ}}) \) matrix that affects rotations in the subspace of degenerate bands. The gauge freedom in \( O(k) \) is fixed, up to trivial \( U(1) \) phase windings, by requiring that the WF’s are maximally localized. [30] Equivalently, we require that the WF’s are eigenfunctions of the projected position operator \( \mathcal{P}_{\text{occ}} \hat{x} \mathcal{P}_{\text{occ}} \): [31]

\[
( \mathcal{P}_{\text{occ}} \hat{x} \mathcal{P}_{\text{occ}} - \frac{1}{2\pi} \vartheta^{(j)} - R ) \Psi^{(j)}(x - R) = 0. \]  

(2.11)

Here, \( \mathcal{P}_{\text{occ}} \) projects to the occupied subspace, and a unit length separates two unit cells. We will shortly derive that the spectrum \( \{ \vartheta^{(j)} \} \) coincide with the phases of the \( W \)-spectrum. Through (2.11) we map the electron density to classical point charges at the positions \( \vartheta^{(j)}/2\pi + R \), for all \( R \); we call these positions the Wannier centers. \( \vartheta = \pi \) corresponds to
a Wannier center that is displaced from the origin by half a unit length. We interchangeably use ‘Wannier center’ and ‘Berry phase’ to mean the same quantity.

The remainder of Sec. 2.2 demonstrates that the phases of the $W$-spectrum coincide with the eigenspectrum of the projected position operator $\mathcal{P}^{\text{occ}} \hat{x} \mathcal{P}^{\text{occ}}$. [31] Here, $\mathcal{P}^{\text{occ}}$ projects to the occupied subspace of the translationally-invariant Hamiltonian (2.1), which have Bloch eigenfunctions $\psi^n_k(x) = e^{ikx} u^n_k(x)$. We are interested in eigenfunctions $\Psi$ that satisfy

$$\left( \mathcal{P}^{\text{occ}} \hat{x} \mathcal{P}^{\text{occ}} - \frac{1}{2\pi} \vartheta \right) \Psi(x) = 0 \quad (2.12)$$

for some eigenvalue $\vartheta/2\pi$. We expand $\Psi$ in the subspace of occupied Bloch waves:

$$\Psi(x) = \sum_{n=1}^{n_{\text{occ}}} \int \frac{dk}{2\pi} f_{nk} \psi^n_k(x). \quad (2.13)$$

In the periodic gauge ($\psi^n_k = \psi^n_{k+2\pi}$), the action of the projected position operator on the wavefunction $f$ may be decomposed into an intra-band operator $\partial_k$ and an inter-band operator $C$: [32]

$$\langle \psi^n_k | \mathcal{P}^{\text{occ}} \hat{x} \mathcal{P}^{\text{occ}} | \Psi \rangle = i \frac{\partial f_{nk}}{\partial k} + i \sum_{m=1}^{n_{\text{occ}}} [C(k)]^{nm} f_{mk}, \quad (2.14)$$

where $C$ is the non-Abelian connection that is defined in (2.5). In the general solution to (2.12), the wavefunctions at two different momenta ($k$ and $k^{(i)}$) are related by the Wilson line

$$f_{mk} = e^{-i(k-k^{(i)})\vartheta/2\pi} \sum_{n=1}^{n_{\text{occ}}} \left[ T e^{-\int_{k^{(i)}}^{k} C(q) dq} \right]^{mn} f_{nk^{(i)}}. \quad (2.15)$$

It follows from the periodic boundary condition on $f$ that

$$\sum_{n=1}^{n_{\text{occ}}} W_{k+2\pi\leftarrow k}^{m} f_{nk} = e^{i\vartheta} f_{m,k+2\pi} = e^{i\vartheta} f_{m,k}, \quad (2.16)$$

hence we have shown that the eigenspectrum of $\mathcal{P}^{\text{occ}} \hat{x} \mathcal{P}^{\text{occ}}$ coincides with the phases of the eigenspectrum of $W$. Furthermore, let us derive the eigenfunctions of $\mathcal{P}^{\text{occ}} \hat{x} \mathcal{P}^{\text{occ}}$. Define the $U(n_{\text{occ}})$ matrix $Q(k)$ such that its columns are the eigenstates of the Wilson loop at base point $k$: $W_{k+2\pi\leftarrow k}$. That is, $W_{k+2\pi\leftarrow k} = Q(k) D Q^\dagger(k)$, where $D$ is a diagonal matrix.
that contains the eigenvalues of $W$. While the eigenvalues of $W$ do not depend on the base point $k$, the eigenfunctions $Q(k)$ do. The matrix $Q(k)$ is related to the matrix $Q(k' \neq k)$ by a Wilson line:

$$
W_{k' + 2\pi \leftarrow k} = W_{k \leftarrow k'}^\dagger W_{k + 2\pi \leftarrow k} W_{k \leftarrow k'}
$$

$$
\Rightarrow Q(k') = W_{k \leftarrow k'}^\dagger Q(k) = W_{k' \leftarrow k} Q(k).
$$

(2.17)

We label the $j$'th diagonal element in $D$ by $\exp(i\vartheta(j))$, where $j$ runs from $1, 2 \ldots n_{\text{occ}}$. If $\vartheta(j)/2\pi$ is an eigenvalue of $P_{\text{occ}} \hat{x} P_{\text{occ}}$, so is any integer addition to $\vartheta(j)/2\pi$, as is consistent with $\vartheta(j)$ being a phase. For each occupied band, there exists an infinite ladder of eigenvalues: $\vartheta_R(j)/2\pi = \vartheta(j)/2\pi + R; R \in \mathbb{Z}$. The index $R$ labels the unit cell where the eigenfunction is localized. We will choose the convention that $-\pi < \vartheta(j) \leq \pi$. Let us then label the eigenfunctions of $P_{\text{occ}} \hat{x} P_{\text{occ}}$ by $j = 1 \ldots n_{\text{occ}}$ and $R \in \mathbb{Z}$. The wavefunction $[f_R^{(j)}]_{n,k} \propto Q(k)_{nj}$ so as to satisfy the eigenvalue equation (2.16). In addition, we multiply the $j$'th column of the eigenmatrix $Q(k)$ by a momentum-dependent phase, so as to ensure periodicity:

$$
[f_R^{(j)}]_{n,k+2\pi} = e^{-i(k+2\pi)\vartheta_R(j)/2\pi} Q(k + 2\pi)_{nj}
$$

$$
eq e^{-i(k+2\pi)\vartheta_R(j)/2\pi} \sum_{m=1}^{n_{\text{occ}}} W_{n,m}^{nm} Q(k)_{mj}
$$

$$= e^{-i(k+2\pi)\vartheta_R(j)/2\pi} e^{i\vartheta_R(j)} Q(k)_{nj} = [f_R^{(j)}]_{n,k}.
$$

(2.18)

In the second equality, we have applied the relation (2.17). In summary, to each eigenvalue $\vartheta_R(j)/2\pi$ there corresponds an eigenfunction of $P_{\text{occ}} \hat{x} P_{\text{occ}}$:

$$
\Psi^{(j)}(x - R) = \sum_{n=1}^{n_{\text{occ}}} \int \frac{dk}{2\pi} e^{i(k(\vartheta_R(j)/2\pi + R) Q(k)_{nj} \psi_R^{(j)}(x)}.
$$

(2.19)

2.3 The Tight-Binding Wilson Loop

As defined in (2.9), the continuum Wilson loop $W$ is expensive to compute numerically. In this Section, we introduce the tight-binding Wilson loop $W_A$, which is computable with
relative ease. We define the tight-binding connection $A$ as

$$A_{mn}^\mu(k) = \langle U_m^k | \frac{\partial}{\partial k_\mu} | U_n^k \rangle,$$  \hspace{1cm} (2.20)

and the tight-binding Wilson loop $W_A$ as the path-ordered exponential of $A$:

$$W_A = T \exp \left[ -\int dq_\mu A_\mu(q) \right].$$  \hspace{1cm} (2.21)

The tight-binding Wilson loop (2.21) and the continuum Wilson loop (2.9) generically have different eigenspectra. Indeed, by inserting the expression for $u_n^k$ into (2.5), we find

$$C_\mu(k) = A_\mu(k) - i [\hat{X}_\mu]^k,$$  \hspace{1cm} (2.22)

with

$$[\hat{X}_\mu]^k_{nm} = \frac{1}{N} \sum_{\alpha\beta} [U^m_{k}]_{\beta} [U^n_{k}]_{\alpha} \sum_{R,R'} e^{ik(R+r^{(\alpha)}-R'-r^{(\beta)})}$$

$$\times \int d^3 r \varphi^*_{\beta}(r-R'-r^{(\beta)})[\varphi_{\alpha}(r-R-\mu) - \varphi_{\alpha}(r-\mu-R')],$$  \hspace{1cm} (2.23)

where $\mu$ denotes a spatial direction. However, both Wilson loops are constrained by the same symmetries and their spectra are expected to share the same topological features. In the remainder of this thesis, we speak only of the tight-binding Wilson loop, which we henceforth denote as $W$.

2.4 Properties of Wilson loops

In this Section we derive several properties of Wilson loops, which apply to both continuum and tight-binding versions, as defined in Sec. 2.1 and 2.3 respectively. The derivations have been carried out with the tight-binding connection $A_k$ (cf. Eq. (2.20) ) and for a 1D BZ; they are trivially generalizable to the continuum connection $C_k$ (cf. Eq. (2.5) ) and to higher dimensions.

(i) The form of $W[l]$ in Eq. (2.21) is applicable to a basis of wavefunctions which is differentiable in $k$. By basis (or gauge), we mean a choice of a set of occupied Bloch wavefunctions
\{u_{i,k}\}, for each momentum along the loop \(l\). Requiring a differentiable basis complicates any numerical computation. We are thus motivated in formulating a discretized expression of \(W[l]\); the discretization amounts to dividing \(l\) into infinitesimally-separated momenta: \(\{k^{(0)} + G, k^{(N-1)}, k^{(N-2)}, \ldots, k^{(2)}, k^{(1)}, k^{(0)}\}\), with \(N \to \infty\) and \(G\) a reciprocal lattice vector. Let us define \(P(k) = \sum_{n_{\text{occ}}=1}^{n_{\text{occ}}} |u_{i,k}\rangle\langle u_{i,k}|\) as the projection to the occupied bands. \(W\) is expressed as path-ordered product of projections, sandwiched by tight-binding eigenfunctions at the base and end points [33], i.e., it has matrix elements

\[
W[l]_{ij} = \langle u_{i,k^{(0)}+G}^{k^{(0)}+G-k^{(0)}} \prod_{\alpha} P(k^{(\alpha)}) |u_{j,k^{(0)}}\rangle.
\]

In this form, differentiability is manifestly not required. Implicit in the definition of \(W[l]\) is our choice of the so-called periodic gauge:

\[
|u_{i,k+G}\rangle = V(G)^{-1} |u_{i,k}\rangle,
\]

where \(V(G)\) encodes the generic non-periodicity of our basis vectors \(\phi_{k,\alpha}\) under \(k \to k + G\), for a reciprocal lattice (RL) vector \(G\); cf. (1.4). It follows that the non-Abelian Berry factors are the unimodular eigenvalues of the operator

\[
\hat{\mathcal{W}} = V(G) \prod_q P(q).
\]

Since each projection is invariant under a \(U(n_{\text{occ}})\) gauge transformation, the eigenspectrum of \(\mathcal{W}\) is manifestly gauge-invariant.

(ii) Let us define the overlap matrix between two momenta by its matrix elements

\[
S(k_1, k_2)_{ij} = \langle u_{i,k_1} | u_{j,k_2} \rangle; \quad i, j \in \{1, 2, \ldots, n_o\}.
\]

A third useful expression of the Wilson loop is as a path-ordered product of overlap matrices:

\[
W[l]_{ij} = \sum_{r_1, r_2, \ldots, r_{N-1}=1}^{n_{\text{occ}}} S(k^{(0)} + G, k^{(N-1)})_{i,r_N-1} S(k^{(N-1)}, k^{(N-2)})_{r_N-1,r_{N-2}} \ldots S(k^{(2)}, k^{(1)})_{r_2,r_1} S(k^{(1)}, k^{(0)})_{r_1,j}
\]
which follows directly from (2.24).

(iii) Let us denote a Wilson line over a path with start point \(k^{(i)}\) and end point \(k^{(f)}\) as \(W_{k^{(f)}\leftarrow k^{(i)}}\). The Wilson line satisfies the unitary condition

\[
W_{k^{(2)}\leftarrow k^{(1)}}(C)^\dagger = W_{k^{(1)}\leftarrow k^{(2)}}(C^T) = W_{k^{(2)}\leftarrow k^{(1)}}(C)^{-1},
\]

where \(C\) is a path that connects two arbitrary momenta \(k^{(1)}\) and \(k^{(2)}\), and \(C^T\) is the same path with reversed orientation. For \(k^{(2)} = k^{(1)} + 2\pi\), the above relation generalizes to Wilson loops. From (2.29) one can derive that for a fixed loop, the eigenspectrum of \(W\) is independent of the base point.

(iv) We briefly comment on the choice of spatial origin. If it is changed, e.g. \(\forall \alpha, \ r_\alpha \rightarrow r_\alpha + \delta\), then \(V(G) \rightarrow V(G) e^{iG \cdot \delta}\) while \(H(k)\) (and consequently \(P(k)\)) is invariant. From (2.26) we deduce that the eigenspectrum of \(W\) is translated by a global \(U(1)\) phase.
Part III

Thesis body
Chapter 3

Spin-Orbit-Free Topological Insulators without Time-Reversal Symmetry

Despite the large number of space groups, there are few known examples of topological boundary modes which are protected by crystal symmetries alone. In this chapter, we explore the 32 crystallographic point groups and identify topological phases of matter with robust surface modes. For $n = 3, 4$ and 6 of the $C_{nv}$ groups, we find the first-known 3D topological insulators (TI’s) without spin-orbit coupling, and with surface modes that are protected only by point groups; our findings differ from past theoretical proposals in not needing time-reversal symmetry (TRS). To describe these $C_{nv}$ systems, we introduce the notions of (a) a halved mirror chirality: an integer invariant which characterizes half-mirror-planes in the 3D Brillouin zone (BZ), and (b) a bent Chern number: the traditional TKNN invariant generalized to bent 2D manifolds (illustrated in Fig. 3.1). We further find that a Weyl semimetallic phase intermediates two gapped phases with distinct halved chiralities.

To date, all experimentally-realized TIs are strongly spin-orbit-coupled, and a variety of exotic phenomenon originate from this coupling, e.g., Rashba spin-momentum locking on
Figure 3.1: Bottom: (a) Half-mirror-planes (HMP’s) in the 3D Brillouin zone (BZ) of a hexagonal lattice with $C_{3v}^{(b)}$ symmetry. Blue face: HMP$_1$. Brown: HMP$_2$. Red: HMP$_3$. (b) HMP’s in the 3D BZ of a tetragonal lattice with $C_{4v}$ symmetry. Red: HMP$_4$. Blue: HMP$_5$. (c) Blue: HMP$_1$ in the 3D BZ of a hexagonal lattice with $C_{6v}$ symmetry. Note that the black-colored submanifold in (c) is not a HMP. In each of (a), (b) and (c), we define a bent Chern number on the triangular pipe with its ends identified. Top: Non-black lines are half-mirror-lines (HML’s) in the corresponding 2D BZ of the 001 surface; each HML connects two distinct $C_m$-invariant points with $m > 2$.

Figure 3.2: (a) Top-down view of hexagonal BZ with $C_{3v}^{(a)}$ symmetry; our line of sight is parallel to the rotational axis. (b) Hexagonal BZ with $C_{3v}^{(b)}$ symmetry. (c) Tetragonal BZ with $C_{4v}$ symmetry. (d) Hexagonal BZ with $C_{6v}$ symmetry. Reflection-invariant planes are indicated by solid lines. Except the line through Γ, all non-equivalent $C_n$-invariant lines are indicated by circles for $n = 2$, triangles for $n = 3$ and squares for $n = 4$. For each of $\{C_{3v}^{(a)}, C_{3v}^{(b)}\}$, there are two independent mirror Chern numbers, defined as $C_e$ ($C_o$) in the mirror-even (odd) subspace. In both (a) and (b), $C_e$ and $C_o$ are defined on a single mirror plane indicated in red; in (b), the two red lines correspond to two projected planes which connect through a reciprocal lattice vector (dashed arrow).

the surface of a TI. [38] Considerably less attention has been addressed to spinless systems, i.e., insulators and semimetals in which spin-orbit coupling is negligibly weak. [19, 36] The topological classifications of spinless and spin-orbit-coupled systems generically differ. A case in point is SnTe, a prototypical $C_{nv}$ system with strong spin-orbit coupling. [7, 39] In SnTe, the mirror Chern number [34] was introduced to characterize planes in the 3D BZ which are invariant under reflection, or mirror planes in short. The Bloch wavefunctions in each mirror plane may be decomposed according to their representations under reflection, and each subspace may exhibit a quantum anomalous Hall effect; [2] we denote $C_e$ ($C_o$)
as the Chern number in the even (odd) subspace of reflection. One may similarly define mirror Chern numbers for spinless $C_{nv}$ systems, as illustrated for $C_{3v}$ in Fig. 3.2(a) and (b). However, for $n = 2, 4$ and 6, such characterization is always trivial due to two-fold rotational symmetry and the lack of spin-orbit coupling, i.e., $C_e = C_o = 0$.

In this chapter, we propose that point-group-protected surface modes can exist without mirror Chern numbers, if the point group satisfies the following criterion: there exist at least two high-symmetry points ($k_1$ and $k_2$) in the surface BZ, which admit two-dimensional irreducible representations (irreps) of the little group [18] at each point. This is fulfilled by crystals with $C_{4v}$ and $C_{6v}$ symmetries, but not $C_{2v}$. There exist in nature two kinds of $C_{3v}$: $C_{3v}^{(a)}$ and $C_{3v}^{(b)}$, which differ in the orientation of their mirror planes; compare Fig. 3.2(a) with (b). Only $C_{3v}^{(b)}$ fulfills our criterion. Henceforth, $C_{nv}$ is understood to mean $C_{3v}^{(b)}$, $C_{4v}$ and $C_{6v}$. We are proposing that surface bands of $C_{nv}$ systems assume topologically distinct structures on lines which connect $k_1$ to $k_2$. We are particularly interested in half-mirror-lines (HML’s), that each satisfies two conditions: (a) It connects two distinct $C_m$-invariant points for $m > 2$; we illustrate this in Fig. 3.1, where a $C_m$-invariant point is mapped to itself under an $m$-fold rotation, up to translations by a reciprocal lattice vector. (b) All Bloch wavefunctions in a HML may be diagonalized by a single reflection operator. On these HML’s, we would like to characterize orbitals that transform in the 2D irrep of $C_{nv}$, e.g., $(p_x, p_y)$ or $(d_{xz}, d_{yz})$ orbitals. We refer to these as the doublet irreps, and all other irreps are of the singlet kind.

\[\chi = 0\] 
\[\chi = -2\] 
\[\chi = -1\] 
\[\chi = 1\] 
\[\chi = 2\]

Figure 3.3: Distinct connectivities of the (001) surface bands along the half-mirror-lines. Black solid (dotted) lines indicate surface bands with eigenvalue +1 (-1) under reflection $M_i$; crossings between solid and dotted lines are robust due to reflection symmetry. For simplicity, we have depicted all degeneracies at momenta $s = 0$ and $s = 1$ as dispersing linearly with momentum. This is true if the little group of the wavevector (at $s \in \{0, 1\}$) is $C_{3v}$, but for $C_{4v}$ and $C_{6v}$ such crossings are in reality quadratic.
We begin by parametrizing HML_i with $s_i \in [0,1]$, where $s_i = 0 \ (1)$ at the first (second) $C_m$-invariant point. The subscript $i$ labels the different HML’s in a $C_{nv}$ system; the $i$’th HML is invariant under a specific reflection $M_i$. At $s_i = 0$ and 1, (001) surface bands form doubly-degenerate pairs with opposite mirror eigenvalues, irrespective of whether the system has TRS. To prove this, let $U(g)$ represent the symmetry element $g$ in the orbital basis. Suppose $U(M_i)\eta = \eta$ for $\eta \in \{\pm 1\}$. By assumption, $|\eta\rangle$ transforms in the doublet representation, i.e., it is a linear combination of states with complex eigenvalues under $U(C_m)$, for $m > 2$. It follows that $[U(C_m) - U(C_m^{-1})] |\eta\rangle$ is not a null vector, and moreover it must have mirror eigenvalue $-\eta$ due to the relation $M_i C_m M_i^{-1} = C_m^{-1}$. Given these constraints at $s_i = 0$ and 1, there are $Z$ ways to connect mirror-even bands to mirror-odd bands, as illustrated schematically in Fig. 3.3. We define the halved mirror chirality $\chi_i \in Z$ as the difference in number of mirror-even chiral modes with mirror-odd chiral modes; if $\chi_i \neq 0$, the surface bands robustly interpolate across the energy gap. $\chi_i$ may be easily extracted by inspection of the surface energy-momentum dispersion: first draw a constant-energy line within the bulk energy gap and parallel to the HML, e.g., the blue line in Fig. 3.3. At each intersection with a surface band, we calculate the sign of the group velocity $dE/ds_i$, and multiply it with the eigenvalue under reflection $M_i$. Finally, we sum this quantity over all intersections along HML_i to obtain $\chi_i$. In Fig. 3.3, we find two intersections as indicated by red squares, and $\chi_i = (1)(1) + (-1)(-1) = 2$. The $Z$-classification of (001) surface bands relies on doublet irreps in the surface BZ; on surfaces which break $C_{nv}$ symmetry, the surface bands transform in the singlet irreps, and cannot assume topologically distinct structures.

Thus far we have described the halved chirality $\chi_i$ as a topological property of surface bands along HML_i, but we have not addressed how $\chi_i$ is encoded in the bulk wavefunctions. Taking $\hat{z}$ to lie along the rotational axis, each HML_i in the surface BZ is the $\hat{z}$-projection of a half-mirror-plane (HMP_i) in the 3D BZ, as illustrated in Fig. 3.1. Each HMP connects two distinct $C_m$-invariant lines for $m > 2$, and all Bloch wavefunctions in a HMP may be diagonalized by a single reflection operator. HMP_i is parametrized by $t_i \in [0,1]$ and
\( k_z \in (-\pi, \pi] \), where \( t_i = 0 \) \((1)\) along the first \((\text{second})\) \( C_m \)-invariant line. Then the halved mirror chirality has the following expression by bulk wavefunctions:

\[
\chi_i = \frac{1}{2\pi} \int_{\text{HMP}_i} dt_i dk_z (F_e - F_o) \in \mathbb{Z}.
\]

For spinless representations, \( M_i^2 = I \), and we label bands with mirror eigenvalue +1 \((-1)\) as mirror-even \((\text{mirror-odd})\). \( F_e \) \((F_o)\) is defined as the Berry curvature of occupied doublet bands, \([27,29]\) as contributed by the mirror-even \((\text{-odd})\) subspace.

For \( C_{3v}^{(b)} \), there exists three independent HMP’s as illustrated in Fig. 3.1-(a), which we label by \( i \in \{1, 2, 3\}\); all other HMP’s are related to these three by symmetry. The \( C_{6v} \) group is obtained from \( C_{3v}^{(b)} \) by adding six-fold rotational symmetry, which enforces \( \chi_2 = 0 \), and \( \chi_1 = -\chi_3 \). The sign in the last identity is fixed by our parametrization of \( \{t_i\} \), which increase in the directions indicated by blue arrows in Fig. 3.2. Thus, HMP1 is the sole independent HMP for \( C_{6v} \). Finally, we find that there are two HMP’s for \( C_{4v} \), labelled by \( i \in \{4, 5\} \) (Fig. 3.1(b)). Unlike the other highlighted HMP’s, HMP5 is the union of two mirror faces, HMP_{5a} and HMP_{5b}, which are related by a \( \pi/2 \) rotation. States in HMP_{5a} are invariant under the reflection \( M_y : y \rightarrow -y \), while in HMP_{5b} the relevant reflection is \( M_x : x \rightarrow -x \). The product of these orthogonal reflections is a \( \pi \) rotation \((C_2)\) about \( \hat{z} \), thus \( M_x = C_2 M_y \). In the doublet representation, all orbitals are odd under a \( \pi \)-rotation, thus \( U(C_2) = -I \) and all states in HMP5 may be labelled by a \emph{single} operator \( M_y \equiv M_5 \).

The invariants \( \{\chi_i\} \) are well-defined so long as bulk states in the HMP’s are gapped, which is true of \( C_{nv} \) insulators. These invariants may also be used to characterize \( C_{nv} \) semimetals, so long as the gaps close away from the HMP’s. Such band touchings are generically Weyl nodes, \([40,41]\) though exceptions exist with a conjunction of time-reversal and inversion symmetries. \([42]\) The chirality of each Weyl node is its Berry charge, which is positive \((\text{negative})\) if the node is a source \((\text{sink})\) of Berry flux. By the Nielsen-Ninomiya theorem, the net chirality of all Weyl nodes in the BZ is zero. \([43]\) To make progress, we divide the BZ into ‘unit cells’, such that the properties of one ‘unit cell’ determine all others by symmetry. As seen in Fig. 3.1, these ‘unit cells’ resemble the interior of triangular pipes; they are known as the orbifolds \( T^3/C_{nv} \). The net chirality of an orbifold can be nonzero, and
is determined by the Chern number on the 2D boundary of the orbifold. As each boundary resembles the surface of a triangular pipe, we call it a bent Chern number. We define $C_{123}, C_{45}$ and $C_6$ as bent Chern numbers for $C^{(b)}_{3v}, C_{4v}$ and $C_{6v}$ respectively. $C^{(b)}_{3v}$ systems in the doublet representation are described by four invariants $(\chi_1, \chi_2, \chi_3, C_{123})$, which are related by parity$[\chi_1 + \chi_2 + \chi_3] = \text{parity}[C_{123}]$. If $\sum_{i=1}^3 \chi_i$ is odd, $C_{123}$ must be nonzero due to an odd number of Weyl nodes within the orbifold, which implies the system is gapless. If the system is gapped, $\sum_{i=1}^3 \chi_i$ must be even. However, the converse is not implied. For $C_{4v}$, a similar relation holds: parity$[\chi_4 + \chi_5] = \text{parity}[C_{45}]$. These parity constraints may be understood in light of a Weyl semimetallic phase that intermediates two gapped phases with distinct halved chiralities. There are four types of events that alter the halved chirality $\chi_i$ of HMP$_i$; we explain how Weyl nodes naturally emerge in the process. (i) Suppose the gap closes between two mirror-even bands in HMP$_i$. Around this band touching, bands disperse linearly within the mirror plane, and quadratically in the direction orthogonal to the plane. Within HMP$_i$, the linearized Hamiltonian around the band crossing describes a massless Dirac fermion in the even representation of reflection. If the mass of the fermion inverts sign, $\int_{H_{MP_i}} F_e/2\pi$ changes by $\eta \in \{\pm 1\}$, implying that
also changes by $\eta$ through (3.1). This quantized addition of Berry flux is explained by a splitting of the band-touching into two Weyl nodes of opposite chirality, and on opposite sides of the mirror face (Fig. 3.4(a)). In analogy with magnetostatics, the initial band touching describes the nucleation of a dipole, which eventually splits into two opposite-charge monopoles; the flux through a plane separating two monopoles is unity. (ii) The same argument applies to the splitting of dipoles in the mirror-odd subspace, which alters $\int_{\text{HMP}_i} F_0/2\pi$ by $\kappa \in \{\pm 1\}$, and $\chi_i$ by $-\kappa$. For (iii) and (iv), consider two opposite-charge monopoles which converge on HMP$_i$ and annihilate, causing $\chi_i$ to change by unity. The sign of this change is determined by whether the annihilation occurs in the mirror-even or odd subspace. As modeled in the Supplementary Material, the transition between two distinct gapped phases is characterized by a transfer of Berry charge between two distinct HMP’s (Fig. 3.4(e)-(g)). In the intermediate semimetallic phase, the experimental implications include Fermi arcs on the (001) surface. [41, 44, 45]

We hope our classification stimulates a search for materials with $C_{nv}$ symmetry. In the second row of Tab. 3.1, we list the topological invariants which characterize $C_{3v}, C_{4v}$ and $C_{6v}$, for bands of any irrep. In addition to the well-known mirror Chern numbers ($C_e, C_o$), we have introduced the bent Chern numbers as a measure of the Berry charge in each orbifold $T^3/C_{nv}$. If the orbital character of bands near the gap is dominated by the doublet irreps, then the halved mirror chirality $\chi_i$ becomes a useful characterization, as seen in the third row of Tab. 3.1. In particular, the mirror Chern numbers of $C_{3v}^{(b)}$ are completely determined by ($\chi_1, \chi_2, \chi_3, C_{123}$). The singlet and doublet irreps of realistic systems are often hybridized. The topological surface bands that we predict here are robust, so long as this hybridization does not close the bulk gap, and if there are no errant singlet surface bands within the gap. [19]

<table>
<thead>
<tr>
<th>$C_{3v}^{(a)}$</th>
<th>$C_{3v}^{(b)}$</th>
<th>$C_{4v}$</th>
<th>$C_{6v}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_e, C_o$</td>
<td>$C_e, C_o$</td>
<td>$C_{45}$</td>
<td>$C_6$</td>
</tr>
<tr>
<td>$C_e, C_o$</td>
<td>$\chi_1, \chi_2, \chi_3, C_{123}$</td>
<td>$\chi_4, \chi_5, C_{45}$</td>
<td>$\chi_1, C_6$</td>
</tr>
</tbody>
</table>
We discuss generalizations of our findings. In addition to materials whose full group is \( C_{nv} \), we are also interested in higher-symmetry materials whose point groups reduce to \( C_{nv} \) subgroups in the presence of a surface, for \( n = 3, 4 \) or 6. We insist that these higher-symmetry point groups have neither (a) a reflection plane that is orthogonal to the principal \( C_n \) axis, nor (b) a two-fold axis that lies perpendicular to the \( C_n \) axis, and parallel to the mirror-plane. The presence of either (a) or (b) imposes \( \chi = C_e = C_o = 0 \) in any (half) mirror-plane of the \( C_{nv} \) system. Only one such higher-symmetry point group exists: \( D_{3d} \) reduces to \( C_{3v} \) on the \( 111 \) surface. [46] Many \( C_{nv} \) systems naturally have TRS, which constrains all \( C_3^{(a)} \) and \( C_3^{(b)} \) invariants in Tab. 3.1 to vanish, with one independent exception for \( C_3^{(b)} \): \( \chi_1 = -\chi_3 \) can be nonzero. TRS does not constrain the invariants of \( C_{4v} \) or \( C_{6v} \).

Our analysis of charge-conserving systems are readily generalized to spinless superconductors which are describable by mean-field theory. Due to the particle-hole redundancy of the mean-field Hamiltonian, the only nonvanishing invariants from Tab. 3.1 belong to \( C_3^{(a)} \) and \( C_3^{(b)} \); among these nonvanishing invariants, the only constraint is \( \chi_1 = \chi_3 \) for \( C_3^{(b)} \).

While we have confined our description to electronic systems without spin-orbit coupling, the halved chirality is generalizable to photonic crystals which are inherently spinless, and also to cold atoms. Finally, we point out that the bent Chern number and the halved chirality are also valid characterizations of spin-orbit-coupled systems with mirror symmetry. In particular, (3.1) applies to representations with spin if we redefine the mirror-even (-odd) bands as having mirror eigenvalues \( +i \) \((-i) \). The implications are left to future work.

The rest of this Chapter supplements the main results that we have just described. We will employ the notation introduced in Sec. 1, where we described how point-group symmetries constrain a tight-binding Hamiltonian, and introduced the notion of little groups. In Sec. 3.1, we formulate the mirror Chern numbers in systems with \( C_{nv} \) symmetry. For electronic systems with negligible spin-orbit coupling, or intrinsically spinless systems, we show that the mirror Chern numbers must vanish for \( C_{2v}, C_{4v} \) and \( C_{6v} \). In Sec. 3.2, we identify the two-dimensional irreducible representations (irreps) of the \( C_{nv} \) groups, then
derive minimal-derivative, effective Hamiltonians for these doublet irreps. In Sec. 3.3, we formulate the halved mirror chirality ($\chi$), prove that it is quantized to integers, and find an equivalent expression with the Berry-Zak phase. Then we identify certain symmetries beyond the $C_{nv}$ group which constrain $\chi$ to vanish. In Sec. 3.4, we formulate the bent Chern numbers, and show how they are related to the mirror Chern numbers and the halved chiralities. In Sec. 3.5, we describe models with nontrivial $\chi$ for the $C_{3v}^{(b)}$, $C_{4v}$ and $C_{6v}$ groups. Finally, in Sec. 3.6 (Sec. 3.7), we explain the role of time-reversal symmetry (particle-hole redundancy) in constraining some of these topological invariants. The last section is applicable to spinless superconductors with $C_{nv}$ symmetry.

3.1 Mirror Chern numbers in systems with $C_{nv}$ symmetry

3.1.1 Definition of mirror Chern numbers, in systems with or without spin-orbit coupling

If an energy gap exists that distinguishes between occupied and unoccupied bands, we may define the Berry vector potential as

$$A(k) = -i \sum_{n \in \text{occ.}} \langle u_{n,k} | \nabla | u_{n,k} \rangle,$$

and the Abelian Berry field as

$$\tilde{F}(k) = \nabla \times A(k).$$

In (3.2), we sum over all occupied bands. In $C_{nv}$ systems, there exist planes in the 3D BZ which are invariant under a certain reflection, up to translations by a reciprocal lattice vector. In each mirror plane (MP$_i$), there exists an operator $X(M_i)$ which represents the reflection $M_i$; $X(M_i)$ represents an element in the group of the mirror plane, as defined in Sec. 1.5. In representations with spin, $X(M_i)^2 = -I$ and the eigenvalues of reflection are $\pm i$; we define the mirror-even (-odd) bands as having mirror eigenvalues $+i$ ($-i$). In representations without spin, $X(M_i)^2 = +I$ and we define the mirror-even (-odd) bands as
having mirror eigenvalues $+1 (-1)$. Mirror-even bands are denoted by the superscript $(e)$, and we may define the mirror-even Berry field $\tilde{\mathcal{F}}(k)_e$ as
\[ \tilde{\mathcal{F}}(k)_e = -i \sum_{n \in \text{occ.even}} \nabla \times \langle u^e_{n,k} \mid \nabla \mid u^e_{n,k} \rangle, \tag{3.4} \]
where we only sum over occupied bands which transform in the even representation of reflection. We similarly define the mirror-odd Berry field $\tilde{\mathcal{F}}(k)_o$. In each $\text{MP}_i$ we denote an infinitesimal, directed area element by $d\Omega$. The even and odd mirror Chern numbers are defined as
\[ C_e = \frac{1}{2\pi} \int_{\text{MP}} d\Omega \cdot \tilde{\mathcal{F}}(k)_e, \quad C_o = \frac{1}{2\pi} \int_{\text{MP}} d\Omega \cdot \tilde{\mathcal{F}}(k)_o. \tag{3.5} \]

3.1.2 The mirror Chern numbers vanish for spinless systems, with either $C_{2v}, C_{4v}$ or $C_{6v}$ symmetry

By spinless systems, we refer either to electronic systems with spin $SU(2)$ symmetry, or to intrinsically spinless systems such as photonic crystals and certain cold atoms. For $C_{nv}$ systems with $n = 2, 4$ or $6$, there exists a two-fold rotational symmetry about the $\hat{z}$ axis. As shown in Sec. 1.2, this symmetry manifests as
\[ U(C_2) H(k) U(C_2)^{-1} = H(D(C_2) \cdot k), \tag{3.6} \]
where $U(C_2)$ represents a two-fold rotation in the orbital basis, and
\[ D(C_2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +1 \end{pmatrix} \tag{3.7} \]
represents a two-fold rotation in $\mathbb{R}^3$. Since the rotation axis lies within the mirror plane $\text{MP}_i$, the element $C_2$ leaves $\text{MP}_i$ invariant, thus $C_2$ belongs to the little group of $\text{MP}_i$. As shown in Sec. 1.5, each element $g$ in this subgroup is represented by an operator $X(g)$, which satisfy requisite algebraic relations that follows from the group structure, e.g., $X(M_i) X(C_2) X(M_i^{-1}) = X(C_2^{-1})$. Since these representations are assumed to be spinless,
$X(C_2)^2 = I$, and $X(C_2)$ commutes with $X(M_i)$. This implies that a mirror-even state at $k$ is mapped to a mirror-even state at $D(C_2)k$, by two-fold symmetry. It follows that the mirror Berry fields are related by

$$\tilde{F}(k)_e = D(C_2) \cdot \tilde{F}(D(C_2) \cdot k)_e, \quad \text{and} \quad \tilde{F}(k)_o = D(C_2) \cdot \tilde{F}(D(C_2) \cdot k)_o. \quad (3.8)$$

There exists Euclidean basis vectors $(\hat{e}_{\parallel, 1}, \hat{e}_{\parallel, 2}, \hat{e}_{\perp})$ which transform under the reflection into $(\hat{e}_{\parallel, 1}, \hat{e}_{\parallel, 2}, -\hat{e}_{\perp})$; the subscript $\parallel$ ($\perp$) denotes a vector that is parallel (perpendicular) to the mirror plane. Since the two-fold rotational axis lies within MP, $D(C_2) \cdot \hat{e}_{\perp} = -\hat{e}_{\perp}$, and

$$\tilde{F}(k)_e \cdot \hat{e}_{\perp} = -\tilde{F}(D(C_2) \cdot k)_e \cdot \hat{e}_{\perp}. \quad (3.9)$$

Since the directed area element $d\Omega$ is parallel to $\hat{e}_{\perp}$, the contributions to the integral (3.5) at $k$ and $D(C_2)k$ are equal in magnitude but opposite in sign. This implies $C_e = 0$, and a similar argument can be made for $C_o = 0$. It should be noted that in spin-orbit-coupled systems, $X(M_i)$ anticommutes with $X(C_2)$, thus $C_e = -C_o$ instead.

### 3.1.3 Mirror Chern numbers in spinless $C_{3v}$ systems

In $C_{3v}$ systems without spin-orbit coupling, two-fold rotational symmetry is absent, thus the mirror Chern numbers need not vanish for the reason stated in Sec. 3.1.2. These invariants might vanish for other reasons: if the $C_{3v}$ system belongs to a larger symmetry group, for which $C_{3v}$ is a subgroup, then $C_e = C_o = 0$ if there exists either of these additional symmetries: (a) a reflection plane that is orthogonal to the principal $C_3$ axis, or (b) a two-fold axis that lies perpendicular to the $C_3$ axis, and parallel to the mirror-plane. The proof is very similar to that in Sec. 3.3.3 and 3.3.4.

### 3.2 $k \cdot p$ analysis of surface bands in spinless $C_{nv}$ systems

Consider a $C_n$-invariant point which is contained in a mirror line in the 001 surface BZ – the little group of the wavevector is $C_{nv}$. We choose a coordinate system such that: (i) the origin lies at the $C_n$-invariant point, (ii) $\hat{z}$ lies along the principal $C_n$ axis, and (ii)
\( \hat{x} \) is parallel to the mirror line, \( \text{i.e.} \), the reflection \( M_y \) transforms \((x, y) \rightarrow (x, -y)\). We consider surface bands that transform in the doublet irrep of \( C_{nv} \). Each doublet irrep comprises two states with distinct, complex-conjugate eigenvalues under an \( n \)-fold rotation; these two states are degenerate because \( M_y C_n M_y^{-1} = C_n^{-1} \). It should be noted that there are no complex eigenvalues under a two-fold rotation, thus our discussion applies to \( n > 2 \).

Applying \( C_n^n = e \) (the identity), we deduce these eigenvalues: \((e^{i2\pi/3}, e^{-i2\pi/3})\) for \( C_{3v} \), and \((i, -i)\) for \( C_{4v} \). For \( C_{6v} \) there are two pairs: \((e^{i2\pi/3}, e^{-i2\pi/3})\) and \((e^{i\pi/3}, e^{-i\pi/3})\). In summary, there is one doublet irrep in each of the groups \( C_{3v} \) and \( C_{4v} \), and two doublet irreps in the group \( C_{6v} \).

### 3.2.1 Doublet irreducible representation of type 1

For the groups \( C_{3v}, C_{4v} \) and \( C_{6v} \), there exists a doublet irrep which transforms as vectors \((x, y)\). We choose a two-dimensional basis in which \( |1\rangle \) transforms as \( x + iy \) and \( |2\rangle \) as \( x - iy \). In this basis, the representations of our symmetry elements are

\[
U(M_y) = \sigma_1, \quad \text{and} \quad U(C_n) = e^{i2\pi \sigma_3/n}. \tag{3.10}
\]

The effective two-band Hamiltonian may be expressed as

\[
H(k) = d(k) I + f(k) \sigma_+ + f(k)^* \sigma_- + g(k) \sigma_3, \tag{3.11}
\]

where \( d(k) \) and \( g(k) \) are real functions, \( f(k) \) is generally complex, and \( \sigma_\pm = \sigma_1 \pm i\sigma_2 \). This Hamiltonian satisfies the symmetry relations

\[
U(M_y) H(k_+, k_-) U(M_y^{-1}) = H(k_-, k_+), \tag{3.12}
\]

\[
U(C_n) H(k_+, k_-) U(C_n^{-1}) = H(k_+ \omega, k_- \omega^*), \tag{3.13}
\]

where \( k_\pm = k_x \pm ik_y \) and \( \omega = \exp[i2\pi/n] \). We expand

\[
d(k) = \sum_{i \geq 0, j \geq 0} d_{ij} k_+^i k_-^j; \quad f(k) = \sum_{i \geq 0, j \geq 0} f_{ij} k_+^i k_-^j; \quad g(k) = \sum_{i \geq 0, j \geq 0} g_{ij} k_+^i k_-^j. \tag{3.14}
\]

\( C_n \) symmetry imposes

\[
d_{ij} = 0 \quad \text{if} \quad \frac{i - j}{n} \notin \mathbb{Z}; \quad f_{ij} = 0 \quad \text{if} \quad \frac{i - j - 2}{n} \notin \mathbb{Z}; \quad g_{ij} = 0 \quad \text{if} \quad \frac{i - j}{n} \notin \mathbb{Z}. \tag{3.15}
\]
$M_y$ symmetry imposes

$$d_{ij} = d_{ji}; \quad f_{ij} \in \mathbb{R}; \quad g_{ij} = -g_{ji}. \quad (3.16)$$

If the group of the wavevector is $C_{3v}$, an expansion of the effective Hamiltonian to second order in $k$ gives

$$d(k) = m + d k_+ k_-; \quad f(k) = a k_- + b k_+^2; \quad g(k) = 0. \quad (3.17)$$

For $C_{4v}$,

$$d(k) = m + d k_+ k_-; \quad f(k) = a k_-^2 + b k_+^2; \quad g(k) = 0. \quad (3.18)$$

For $C_{6v}$,

$$d(k) = m + d k_+ k_-; \quad f(k) = b k_+^2; \quad g(k) = 0. \quad (3.19)$$

All coefficients $\{m, d, a, b\}$ are real.

### 3.2.2 Doublet irreducible representation of type 2

For the group $C_{6v}$, there exists a second doublet irrep which transforms as $(x^2 - y^2, 2xy)$. We choose the same coordinates as in Sec. 3.2.1, and a two-dimensional basis in which $|1\rangle$ transforms as $(x^2 - y^2) + i2xy$ and $|2\rangle$ as $(x^2 - y^2) - i2xy$. In this basis, the representations of our symmetry elements are

$$U(M_y) = \sigma_1, \quad \text{and} \quad U(C_6) = e^{i2\pi \sigma_3/3}. \quad (3.20)$$

The two-band effective Hamiltonian satisfies the symmetry relations

$$U(M_y) H(k_+, k_-) U(M_y^{-1}) = H(k_-, k_+), \quad (3.21)$$
$$U(C_6) H(k_+, k_-) U(C_6^{-1}) = H(k_+ \omega, k_- \omega^*), \quad (3.22)$$

where $k_\pm = k_x \pm ik_y$ and $\omega = \exp[i2\pi/6]$. $C_6$ symmetry imposes

$$d_{ij} = 0 \quad \text{if} \quad \frac{i-j}{6} \notin \mathbb{Z}; \quad f_{ij} = 0 \quad \text{if} \quad \frac{i-j-4}{6} \notin \mathbb{Z}; \quad g_{ij} = 0 \quad \text{if} \quad \frac{i-j}{6} \notin \mathbb{Z}. \quad (3.23)$$
$M_y$ symmetry imposes the same constraints as in (3.16). An expansion of the effective Hamiltonian to second order in $k$ gives

$$d(k) = m + d k_+ k_-; \quad f(k) = a k^2; \quad g(k) = 0.$$  \hspace{1cm} (3.24)

All coefficients \{m, d, a\} are real.

### 3.3 The halved mirror chirality

#### 3.3.1 Integer quantization of the halved mirror chirality

Let us prove that $\chi \in \mathbb{Z}$, for systems with or without spin-orbit coupling. From the definition (1), we separate $\chi$ into two parts: $2\pi \chi = B_e - B_o$, where

$$B_\eta = \int_{HMP} dt \, dk_z \, \mathcal{F}_\eta(t, k_z),$$  \hspace{1cm} (3.25)

and $\eta \in \{e, o\}$ distinguishes the mirror-even and mirror-odd subspaces, as defined in Sec. 3.1. The Berry curvature in a mirror subspace is defined by

$$\mathcal{F}_\eta(t, k_z) = \partial_t A^\eta(t, k_z) - \partial_z A^\eta(t, k_z)$$  \hspace{1cm} (3.26)

where $\partial_t = \partial/\partial t$, $\partial_z = \partial/\partial k_z$, and

$$A^\eta(t, k_z) = -i \sum_{n \in \text{occ, } \eta} \langle u_{n, (t, k_z)}^\eta | \partial_\mu | u_{n, (t, k_z)}^\eta \rangle.$$  \hspace{1cm} (3.27)

Here we only sum over occupied bands in the representation of reflection denoted by $\eta$. If $\hat{e}_\perp$ is the unit vector orthogonal to HMP, then $\mathcal{F}_\eta = \tilde{\mathcal{F}}_\eta \cdot \hat{e}_\perp$ is a scalar, in comparison with the vector $\tilde{\mathcal{F}}_\eta$ which is defined in Sec. 3.1. In terms of $\mathcal{A}$,

$$B_\eta = \int_0^1 dt \, \partial_t \int_{-\pi}^\pi dk_z A^\eta_z - \int_{-\pi}^\pi dk_z \partial_z \int_0^1 dt \, A^\eta_t.$$  \hspace{1cm} (3.28)

Since $B_\eta$ is expressed in terms of Berry curvature, it is manifestly gauge-invariant. Given that $|u_{n, (t, k_z)}\rangle$ is an eigenstate of $H(t, k_z)$ in the HMP, it follows from (1.8) that $V(2\pi \hat{z})^{-1} |u_{n, (t, k_z)}\rangle$ is an eigenstate of $H(t, k_z + 2\pi)$, up to a $U(1)$ phase ambiguity. It is convenient to choose this arbitrary phase to vanish as

$$|u_{n, (t, k_z + 2\pi)}\rangle = V(2\pi \hat{z})^{-1} |u_{n, (t, k_z)}\rangle,$$  \hspace{1cm} (3.29)
or equivalently \( \psi_{n,(t,k_z)}(r) = \psi_{n,(t,k_z+2\pi)}(r) \). In this periodic gauge, the second term of (3.28) vanishes. The remaining expression may be expressed in terms of the Wilson loop, which is a matrix representation of holonomy. Let us consider the parallel transport of a mirror-eigenstate, around a non-contractible loop in the HMP – at constant \( t \) but varying \( k_z \). In the orbital basis, such transport is represented by the operator

\[
\hat{W}_\eta(t) = V(2\pi \hat{z}) \prod_{k_z} P_\eta(t, k_z),
\]

(3.30)

where \( P_\eta(t, k_z) \) projects into the occupied subspace in the \( \eta \)-representation of reflection:

\[
P_\eta(t, k_z) = \sum_{n \in \text{occ}} \langle u_\eta^n, (t, k_z) | \langle u_\eta^n, (t, k_z) |
\]

(3.31)

and \((\pi \leftrightarrow -\pi)\) indicates that the product of projections is path-ordered. In the basis of \( n_{\text{occ},\eta} \) occupied bands in the \( \eta \)-representation, this same parallel transport is represented by an \( n_{\text{occ},\eta} \times n_{\text{occ},\eta} \) matrix:

\[
[W_\eta(t)]_{ij} = \langle u_\eta^j, (t, -\pi) | \hat{W}_\eta(t) | u_\eta^i, (t, -\pi) \rangle,
\]

(3.32)

where the total eigenspectrum of (3.32) comprise the unimodular eigenvalues of (3.30). It is shown in Ref. [33] that (3.28) may be expressed as

\[
B_\eta = \int_0^1 dt \partial_t \int_{-\pi}^\pi dk_z A_\eta^z = -i \int_0^1 dt \partial_t \ln \det W_\eta(t)
\]

\[
= -i \ln \det W_\eta(t = 1) + i \ln \det W_\eta(t = 0) + 2\pi N_\eta; \quad N_\eta \in \mathbb{Z}.
\]

(3.33)

Here we have chosen the principal branches of the logarithm at endpoints \( t = 0 \) and \( t = 1 \), and \( N_\eta \) is the number of windings in the interval \( t \in (0,1) \), relative to these principal values. We claim that the eigenspectrum of \( W_\eta(t = 0) \) is degenerate with the eigenspectrum of \( W_{-\eta}(t = 0) \), and a similar degeneracy occurs at the other endpoint \( t = 1 \).

Proof: let \( \bar{t} \) denote an endpoint \( t \in \{0,1\} \). The lines at constant \( \bar{t} \) are invariant under (i) a certain \( m \)-fold rotation \((m = 3 \text{ for } C_{3v} \text{ and } C_{6v}, \ m = 4 \text{ for } C_{4v})\), and (ii) a reflection \( M_i \). The set of elements which leave this line invariant form the group of the line; they
are represented by \( \{ X(M_i), X(C_m), X(C_m^{-1}), \ldots \} \), as discussed in Sec. 1.5. The relevant symmetry relations are

\[
\forall \ k_z, \quad [X(C_m), H(\bar{t}, \bar{k}_z)] = [X(C_m^{-1}), H(\bar{t}, \bar{k}_z)] = [X(M_i), H(\bar{t}, \bar{k}_z)] = 0. \tag{3.34}
\]

Analogous to the construction of (3.31) and (3.32), we may define, for all \( n_{occ} \) occupied bands, a \( n_{occ} \times n_{occ} \) Wilson-loop matrix:

\[
[W(\bar{t})]_{ij} = \langle u_{i,(\bar{t},-\pi)} | V(2\pi \hat{\varphi}) \prod_{k_z}^{\pi - \pi} (P_\eta(\bar{t}, k_z) + P_{-\eta}(\bar{t}, k_z)) | u_{j,(\bar{t},-\pi)} \rangle \\
= \langle u_{i,(\bar{t},-\pi)} | \hat{W}(\bar{t}) | u_{j,(\bar{t},-\pi)} \rangle. \tag{3.35}
\]

We also define the complete projection into the occupied bands as \( P = P_\eta + P_{-\eta} \), which projects onto both mirror-odd and -even bands. Since the bands transform in the doublet irreps, \( n_{occ,\eta} + n_{occ,-\eta} = n_{occ} \), as assumed in the main text. Since the mirror subspaces are orthogonal, the eigenspectrum of \( W(\bar{t}) \) comprise the eigenvalues of \( W_\eta(\bar{t}) \) and \( W_{-\eta}(\bar{t}) \). Suppose \( |\eta\rangle \) belongs to the occupied subspace at momentum \( (\bar{t}, k_z = -\pi) \), and the state satisfies two conditions: (i) it is an eigenstate of \( W(\bar{t}) \): \( \hat{W}(\bar{t}) |\eta\rangle = e^{i\varphi} |\eta\rangle \), and (ii) it is also an eigenstate of reflection: \( X(M_i) |\eta\rangle = |\eta\rangle \). It follows from (3.34) that \( X(C_m) |\eta\rangle \) and \( X(C_m^{-1}) |\eta\rangle \) belong in the occupied subspace at \( (\bar{t}, k_z = -\pi) \). Since |\eta\rangle transforms in the doublet irrep, it is a linear combination of states \( \{|\lambda\rangle, |\lambda^*\rangle\} \) with complex eigenvalues under \( X(C_m) \) (for \( m > 2 \)). Note that if \( X(C_m) |\lambda\rangle = \lambda |\lambda\rangle \) for complex \( \lambda \), then \( X(C_m^{-1}) |\lambda\rangle = \lambda^* |\lambda\rangle \neq X(C_m) |\lambda\rangle \). Thus we deduce that \( (X(C_m) - X(C_m^{-1})) |\eta\rangle \) is not a null vector. Then

\[
X(M_i) X(C_m) X(M_i^{-1}) = X(C_m^{-1}) \\
\Rightarrow X(M_i) \left( X(C_m) - X(C_m^{-1}) \right) |\eta\rangle = -\eta \left( X(C_m) - X(C_m^{-1}) \right) |\eta\rangle, \tag{3.36}
\]

\( i.e., \) \(|\eta\rangle \) and \( (X(C_m) - X(C_m^{-1})) |\eta\rangle \) have opposite mirror eigenvalues. From (3.34), we derive

\[
\forall \ k_z, \quad X(C_m) P(\bar{t}, \bar{k}_z) X(C_m^{-1}) = P(\bar{t}, \bar{k}_z). \tag{3.37}
\]

Combining this relation with (1.41) and (3.35),

\[
\hat{W}(\bar{t}) \left( X(C_m) - X(C_m^{-1}) \right) |\eta\rangle = e^{i\varphi} \left( X(C_m) - X(C_m^{-1}) \right) |\eta\rangle. \tag{3.38}
\]
This proves the double-degeneracy in the Wilson-loop spectrum, or equivalently,

\[ \ln \det \mathcal{W}_\eta(\vec{t}) = \ln \det \mathcal{W}_{-\eta}(\vec{t}). \]  

(3.39)

Combining this with (3.33) and (1), we find

\[ \chi_i = \frac{N_\eta - N_{-\eta}}{2\pi} \in \mathbb{Z}, \]  

(3.40)

where \( \eta = 1 \) for spinless representations, and \( i \) for representations with spin.

### 3.3.2 Expressing the halved-mirror chirality with Berry-Zak phases

![Figure 3.5: (a) (resp. (c)) is the 001-surface dispersion (resp. Berry-phase spectrum) of the \( C_{4v} \) topological insulator, with \( \chi = 2 \). (b) and (d) describe a trivial \( C_{4v} \) insulator with \( \chi = 0 \). Along the HML connecting \( \Gamma \) and \( \bar{M} \), mirror-even (resp. odd) surface bands are highlighted in red (resp. blue). Similarly, the Berry phase of the mirror-even (resp. odd) subspace is colored red (resp. blue).](image)

To express (3.1) in terms of Berry phases, we consider a family of non-contractible loops \( \{z(\vec{k}_s)\} \) which lie within the HMP; an example of a loop is illustrated in red in Fig. 3.6(a).

Denoting the eigenvalues of \( \mathcal{W}[z(\vec{k}_s)] \) by \( \{\exp(i\vartheta(\vec{k}_s))\} \), we plot the Berry phases \( \{\vartheta\} \) as a function of \( \vec{k}_s \) in Fig. 3.5(c). Due to the orthogonality of the mirror subspaces, we may label each branch of \( \vartheta \) by its mirror eigenvalue: \( \vartheta_e \) (\( \vartheta_o \)) in the even (odd) subspace is colored red (blue). By Stoke’s theorem, we rewrite (3.1) as the net change in \( \vartheta_e \) in the interval \( s \in [0, 1] \), minus the net change in \( \vartheta_o \):

\[ \chi = \frac{1}{2\pi} \int_0^1 ds \left( \frac{\partial \vartheta_e}{\partial s} - \frac{\partial \vartheta_o}{\partial s} \right). \]  

(3.41)
Since $\vartheta_e = \vartheta_o$ at $s = 0$ and $s = 1$, $\chi$ is quantized to integers – each nonzero integer characterizes a topologically distinct type of spectral flow. $\chi$ may be extracted from $\{\vartheta\}$ in a manner that is analogous to the surface-band index: by considering the intersections of $\{\vartheta\}$ with an arbitrary constant-phase line. At each intersection, we evaluate \[\text{sign of } \frac{d\vartheta}{ds} \times \text{[mirror eigenvalue]},\] then sum this quantity over all intersections along the HML. By inspection of Fig. 3.5(c), we find $\chi = 2$, in one-to-one correspondence with the surface-band formulation of $\chi$. For comparison, we plot the surface bands and Berry phases of a trivial insulator in Fig. 3.5(b) and (d); these are obtained from (7.3) with parameters $n_z = 2$, $\delta = 0.1$ and $\alpha = \beta = 1$. The formula (3.41) is applicable to the case of two occupied bands, as in the model (7.3); to generalize to $2m$ occupied bands for $m > 1$, we interpret $\vartheta_e (\vartheta_o)$ as the sum of all Berry phases in the even (odd) subspace.

3.3.3 $\chi = 0$ with a reflection plane orthogonal to the principal $C_n$ axis

All Bloch wavefunctions in HMP$_i$ may be diagonalized by a single operator, which represents the reflection $M_i$. Suppose there exists another reflection symmetry $M_z$: $z \to -z$, for $\hat{z}$ along the principal $C_n$ axis. Since $M_i$ and $M_z$ are reflections in perpendicular planes, their operations commute. This implies that a mirror-even state at $\mathbf{k}$ is mapped to a mirror-even state at $D(M_z)\mathbf{k}$, hence the mirror Berry curvatures are related by $\mathcal{F}_e(t, k_z) = -\mathcal{F}_e(t, -k_z)$. Similarly, $\mathcal{F}_o(t, k_z) = -\mathcal{F}_o(t, -k_z)$. In comparison with (3.8), there is an extra minus sign
because the Berry field $\tilde{F}$ is a pseudovector, and $D(M_z)$ is an improper rotation. From (3.25), it follows that $B_e = B_o = \chi = 0$.

### 3.3.4 $\chi = 0$ with a two-fold axis that lies perpendicular to the principal $C_n$ axis, and parallel to the half-mirror-plane

Suppose there exists a two-fold rotational symmetry $C_2$, with axis perpendicular to the principal $C_n$ axis, and parallel to HMP$_i$. For spinless representations, $M_i C_2 M_i^{-1} = C_2^{-1} = C_2$, thus their operations commute. This implies that a mirror-even state at momentum $(t, k_z)$ within HMP$_i$ is mapped to a mirror-even state at $(t, -k_z)$ by the two-fold symmetry, hence the mirror Berry curvatures are related by $F_e(t, k_z) = -F_e(t, -k_z)$. Similarly, $F_o(t, k_z) = -F_o(t, -k_z)$. From (3.25), it follows that $B_e = B_o = \chi = 0$.

### 3.4 Relations between the halved mirror chirality and the bent Chern numbers

![Figure 3.7: Top-down view of 3D BZ’s with various symmetries; our line of sight is parallel to the rotational axis. Reflection-invariant planes are indicated by solid lines. Each half-mirror-plane (HMP$_i$) is illustrated by a solid line that connects two distinct $C_m$-invariant lines for $m > 2$. HMP$_i$ is labelled by a number $i$ over the solid line. Arrows that emanate from each HMP indicate the convention in which Berry flux is calculated, i.e., they define in vs out. (a) Tetragonal BZ with $C_{4v}$ symmetry. (b) Hexagonal BZ with $C_{3v}^{(b)}$ symmetry.](image-url)
3.4.1 The halved mirror chirality and the bent Chern number in $C_{4v}$ systems

The halved chiralities and the bent Chern number are related by

\[
\text{parity}[\chi_4 + \chi_5] = \text{parity}[\mathcal{C}_{45}]. \tag{3.42}
\]

Proof: for $i \in \{4, 5\}$, define the mirror Berry flux through HMP$_i$ as

\[
B^{(i)}_{\eta} = \int_{\text{HMP}_i} dt_i \, dk_z \, F_{\eta}(t_i, k_z), \tag{3.43}
\]

where $\eta \in \{e, o\}$ distinguishes between mirror-even and mirror-odd subspaces; $F_{\eta}$ is defined in (3.26) and (3.27). We choose the convention that this flux emanates from the inside of the triangular pipe, as illustrated in Fig. 3.7(a). The total Berry flux is defined $B^{(i)} = B^{(i)}_e + B^{(i)}_o$, and the bent Chern number satisfies $2\pi \mathcal{C}_{45} = B^{(4)} + B^{(5)}$. The halved chiralities are defined by $2\pi \chi_i = B^{(i)}_e - B^{(i)}_o$, thus

\[
\mathcal{C}_{45} = \chi_4 + \chi_5 + \frac{2(B^{(4)}_o + B^{(5)}_o)}{2\pi}. \tag{3.44}
\]

(3.42) follows from proving

\[
\frac{B^{(4)}_o + B^{(5)}_o}{2\pi} \in \mathbb{Z}, \tag{3.45}
\]

which we now do. As in (3.33), we express $B$ in terms of the Wilson loop:

\[
B^{(i)}_o = -i \ln \det \mathcal{W}_{M_i=\eta}(t_i = 1) + i \ln \det \mathcal{W}_{M_i=\eta}(t_i = 0) + 2\pi N^{(i)}; \quad N^{(i)} \in \mathbb{Z}. \tag{3.46}
\]

The subscript $M_i = \eta$ means that $\mathcal{W}$ represents the parallel transport of a state with eigenvalue $\eta$ under $X(M_i)$; $\eta = -1 \ (-i)$ for representations without (with) spin. With our chosen flux conventions, the lines labelled by $t_4 = 0$ and $t_5 = 1$ coincide, and they project to $\bar{\Gamma}$ in the 001 surface BZ, as illustrated in Fig. 1; the lines $t_4 = 1$ and $t_5 = 0$ coincide, and they project to $\bar{M}$ in the surface BZ. We rewrite (3.46) as

\[
B^{(4)}_o = -i \ln \det \mathcal{W}_{M_4=\eta}(\bar{M}) + i \ln \det \mathcal{W}_{M_4=\eta}(\bar{\Gamma}) + 2\pi N^{(4)}; \quad N^{(4)} \in \mathbb{Z},
\]

\[
B^{(5)}_o = -i \ln \det \mathcal{W}_{M_5=\eta}(\bar{\Gamma}) + i \ln \det \mathcal{W}_{M_5=\eta}(\bar{M}) + 2\pi N^{(5)}; \quad N^{(5)} \in \mathbb{Z}. \tag{3.47}
\]
Now we will prove that the eigenspectrum of $W_{M_4=\eta(\bar{k})}$ is identical to that of $W_{M_5=\eta(\bar{k})}$, for both $\bar{k} = \bar{M}$ and $\bar{\Gamma}$. We recall that $M_4$ reflects $(x, y) \rightarrow (y, x)$ and $M_5$ reflects $(x, y) \rightarrow (x, -y)$, thus the product is a four-fold rotation: $C_4 = M_4M_5$, or equivalently their representations satisfy $X(C_4) = X(M_4)X(M_5)$. Suppose $X(M_5)|\eta_5\rangle = \eta_5|\eta_5\rangle$. For spinless representations, it follows from $X(M_4)^2 = X(M_5)^2 = I$ and $X(C_4) = X(M_4)X(M_5)$, that $(I + X(C_4))|\eta_5\rangle$ is an eigenstate of $X(M_4)$ with eigenvalue $\eta_5$. Moreover, since $|\eta_5\rangle$ transforms in the doublet irrep, $(I + X(C_4))|\eta_5\rangle$ is not a null vector. Then we can show that

$$\ln \det W_{M_4=\eta(\bar{k})} = \ln \det W_{M_5=\eta(\bar{k})},$$

in similar fashion to the steps preceding (3.39). For representations with spin, we consider instead $(I - X(C_4))|\eta_5\rangle$, and arrive at the same conclusion. Finally, (3.45) is proven through

$$B^{(4)}_{\eta} = -i \ln \det W_{M_5=\bar{M}} + i \ln \det W_{M_5=\bar{\Gamma}} + 2\pi N^{(4)}$$

$$= -B^{(5)}_{\eta} + 2\pi N^{(5)} + 2\pi N^{(4)}.$$ (3.49)

### 3.4.2 The halved mirror chirality and the bent Chern number in $C_{3v}^{(b)}$ systems

In addition to HMP’s defined in the main text, it is convenient to define HMP$_6$ and HMP$_7$ as illustrated in Fig. 3.7(b). For $i \in \{1, 2, 3, 6, 7\}$, define the mirror Berry flux through HMP$_i$ as

$$B^{(i)}_{\eta} = \int_{\text{HMP}_i} dt_i dk_z F_{\eta}(t_i, k_z),$$

where $\eta \in \{e, o\}$ distinguishes between mirror-even and mirror-odd subspaces; $F_{\eta}$ is defined in (3.26) and (3.27). Our flux conventions are illustrated in the same figure. In HMP$_i$, all states are diagonalized by the reflection $M_i$, and the various reflection operators are related by a three-fold rotation in coordinates: $M_3 = C_3^{-1}M_1C_3$, $M_2 = C_3^{-1}M_3C_3$, etc. The mirror Chern numbers are defined as

$$2\pi C_{\eta} = B^{(7)}_{\eta} + B^{(1)}_{\eta} + B^{(6)}_{\eta}.$$ (3.51)
The halved mirror chiralities are defined as

\[ 2\pi \chi_i = B_e^{(i)} - B_d^{(i)}; \quad i \in \{1, 2, 3\}. \]  

(3.52)

The bent Chern number is defined as

\[ 2\pi C_{123} = \sum_{\eta \in \{e, o\}} \left( B_{\eta}^{(1)} + B_{\eta}^{(2)} + B_{\eta}^{(3)} \right). \]  

(3.53)

Due to the three-fold rotational symmetry,

\[ B_{\eta}^{(6)} = B_{\eta}^{(2)}, \quad \text{and} \quad B_{\eta}^{(7)} = B_{\eta}^{(3)}. \]  

(3.54)

Combining this with (3.51) and (3.53), we find

\[ C_{123} = C_e + C_o. \]  

(3.55)

Combining (3.54) with (3.52) and (3.53), we find

\[ \chi_1 + \chi_2 + \chi_3 = C_e - C_o. \]  

(3.56)

Once we specify \((\chi_1, \chi_2, \chi_3, C_{123})\), the mirror Chern numbers are determined through the relations (3.55) and (3.56). As a corollary,

\[ \text{parity}[\chi_1 + \chi_2 + \chi_3] = \text{parity}[C_{123}]. \]  

(3.57)

### 3.5 Models

#### 3.5.1 Modelling a \(C_{4v}\) system

To exemplify our theory, we consider a \(C_{4v}\) model on a tetragonal lattice, which comprises two interpenetrating cubic sublattices. The Bloch Hamiltonian is

\[
H(k) = \left[ -1 + 8 f_1(k) \right] \Gamma_{03} + C f_2(k) \Gamma_{01} + 2 f_3(k) \Gamma_{11} \\
+ E f_4(k) \Gamma_{32} + 2 f_5(k) \Gamma_{12},
\]

(3.58)

where \(f_1 = 3 - \cos(k_x) - \cos(k_y) - \cos(k_z)\), \(f_2 = \cos(k_y) - \cos(k_x)\), \(f_3 = 2 - \cos(k_x) - \cos(k_y)\), \(f_4 = \sin(k_x) \sin(k_y)\) and \(f_5 = \sin(k_z)\). We define \(\Gamma_{ab} = \sigma_a \otimes \tau_b\), where \(\sigma_i\) and \(\tau_i\) are Pauli...
Figure 3.8: (a) Phase diagram of $C_{4v}$ model (3.58); $C$ and $E$ are varied to induce phase transitions. Blue (uncolored) regions correspond to gapped (gapless) phases. The halved chiralities in each phase are indicated by two integers: $(\chi_4,\chi_5)$. The blue square in the center is approximately bounded by $|C| < 2$ and $|E| < 2$. (b) Bulk dispersion of the semimetallic phase; $(\chi_4,\chi_5) = (0, -1)$. (c) Surface dispersions along $M - \Gamma - X$. Top of (c): semimetal with $(\chi_4,\chi_5) = (0, -1)$. Bottom: TI with $(\chi_4,\chi_5) = (-1, -1)$.

matrices for $i \in \{1, 2, 3\}$; $\sigma_0$ and $\tau_0$ are identities in each 2D subspace. $|\sigma_3 = \pm 1, \tau_3 = +1\rangle$ label $\{p_x \pm ip_y\}$ orbitals on one sublattice, and $|\sigma_3 = \pm 1, \tau_3 = -1\rangle$ label $\{p_x \mp ip_y\}$ orbitals on the other. This Hamiltonian has the four-fold symmetry: $\Gamma_{33} H(k_x, k_y, k_z) \Gamma_{33} = H(-k_y, k_x, k_z)$, and the reflection symmetry: $\Gamma_{10} H(k_x, k_y, k_z) \Gamma_{10} = H(k_x, -k_y, k_z)$. A phase diagram is plotted in Fig. 3.8(a) for different parametrizations of (3.58); the sweep of parameters indicated by the red line produces the Weyl trajectories of Fig. 4(e). In Fig. 3.8(b) and (c) we illustrate the energy dispersions at two points along this sweep.

### 3.5.2 Modelling $C_{3v}^{(b)}$ and $C_{6v}$ systems

We model a $C_{3v}^{(b)}$ system on a hexagonal lattice composed of two interpenetrating triangular sublattices. Defining $k_1 = \mathbf{k} \cdot \mathbf{a}_1$ and $k_2 = \mathbf{k} \cdot \mathbf{a}_2$, with $\mathbf{a}_1 = (1, 0, 0)$ and $\mathbf{a}_2 = (-1/2, \sqrt{3}/2, 0)$, the Hamiltonian is

$$H(\mathbf{k}) = \left[ \frac{5}{2} - \cos(k_1 + \phi) - \cos(k_2 + \phi) - \cos(k_1 + k_2 - \phi) - \cos(k_2) \right] \Gamma_{30} + \Gamma_{10}$$

$$+ \left\{ z \left[ e^{i\pi/3} \cos k_1 + e^{-i\pi/3} \cos k_2 - \cos(k_1 + k_2) \right] \Gamma_{1+} + h.c. \right\} + \sin(k_z) \Gamma_{20} \quad (3.59)$$

with $\phi = 2\pi/3$. $\Gamma_{1+} = \sigma_1 \otimes (\tau_1 + i\tau_2)$. $\sigma_3 = \pm 1$ label the two sublattices, and $\tau_3 = \pm 1$ label the $\{p_x \pm ip_y\}$ orbitals. $C_3$ symmetry manifests as

$$X(C_n) H(\mathbf{k}) X(C_n)^{-1} = H(D(C_n)\mathbf{k}), \quad (3.60)$$
for $n = 3$; $X(C_3) = \sigma_0 \otimes \exp(i 2\pi \tau_3/3)$, and $D(C_n)$ represents an $n$-fold rotation in $\mathbb{R}^3$. The reflection symmetries include $\Gamma_0 1 H(k) \Gamma_0 1 = H(R(M_3)k)$, where $D(M_3)$ represents a reflection across the mirror plane intersecting HMP$_3$. $z = 0.25$ describes a gapped phase with trivial $\{\chi_i\}$. As we tune $z$ from 0.25 to 0.3, a Berry dipole nucleates in HMP$_2$, then splits into two monopoles with opposite charge; this semimetallic phase is described by $\chi_1 = 0, \chi_2 = 1, \chi_3 = 0$ and $C_{123} = 1$; cf. (3.57). As $z$ is further increased to 0.5, pairs of monopoles converge on HMP$_1$ and annihilate. The resultant gapped phase satisfies $\chi_1 = 1, \chi_2 = 1, \chi_3 = 0$. This process is depicted in Fig. 4(f). In our final example, we set $\phi = 0$ in (3.59) so that the Hamiltonian additionally satisfies the symmetry relation (3.60) for $n = 6$ and $U(C_6) = \sigma_0 \otimes \exp(i \pi \tau_3/3)$. $z = 0.5$ describes a trivial gapped $C_6v$ phase, and increasing $z$ to 0.75 produces a gapped phase with $\chi_1 = -1$; the intermediate Weyl trajectories are illustrated in Fig. 4(g).

### 3.6 Additional constraints on topological invariants due to time-reversal symmetry

In spinless systems, time-reversal symmetry (TRS) constrains $C_e = C_o = 0$ in $C_{3v}^{(a)}$ systems, $\chi_1 = -\chi_3$ and $\chi_2 = C_e = C_o = 0$ in $C_{3v}^{(b)}$ systems; no analogous constraints exist for $C_{4v}$ or $C_{6v}$.

#### 3.6.1 Time-reversal symmetry in spinless $C_{3v}^{(a)}$ systems

Let $T$ denote the spinless time-reversal operation, and $M$ denote a reflection in the mirror plane (MP) colored red in Fig. 2(a). Let $k$ be a momentum within MP. Since $[T,M] = 0$ and the reflection eigenvalues are real for spinless representations, a state in the even representation at $k$ is mapped by time-reversal to a state in the even representation at $-k$, which also lies in MP. It follows that the mirror Berry curvatures are related by $F_e(k) = -F_e(-k)$, and the net contribution to the integral in (3.5) is zero, thus $C_e = 0$. Similarly, $F_o(k) = -F_o(-k)$ implies $C_o = 0$. 
3.6.2 Time-reversal symmetry in spinless $C_{3v}^{(b)}$ systems

The proof is similar to that in Sec. 3.6.1. Time-reversal ($T$) relates states within HMP$_2$, and imposes $B_e^{(2)} = B_o^{(2)} = 0$, as defined in (3.50). A product of time-reversal and a three-fold rotation relates states in HMP$_1$ to states in HMP$_3$, thus $B_e^{(1)} = -B_e^{(3)}$, and $B_o^{(1)} = -B_o^{(3)}$. The conclusion is that $\chi_1 = -\chi_3$ and $\chi_2 = C_e = C_o = C_{123} = 0$.

3.6.3 Time-reversal symmetry in spinless $C_{4v}$ and $C_{6v}$ systems

The following discussion applies to any HMP$_i$ in either $C_{4v}$ or $C_{6v}$ systems. A product of time-reversal and a two-fold rotation relates states within the same HMP$_i$ as: $F_\eta(t_i, k_z) = F_\eta(t_i, -k_z)$, for both mirror-even and -odd subspaces; the parametrization $(t_i, k_z)$ is defined in the main text. This relation does not constrain any of the above-mentioned topological invariants.

3.7 Generalization to spinless superconductors

The mirror Chern numbers, bent Chern numbers and halved mirror chirality are readily generalized to mean-field Hamiltonians in the Bogoliubov-de Gennes (BdG) formalism. If Hermitian, the BdG Hamiltonian has a particle-hole redundancy:

$$PH(k)P^{-1} = -H(-k)$$

for an antiunitary operator $P$. This relation imposes certain constraints on our topological invariants. If there exists a two-fold rotational symmetry about the principal rotation axis of $C_{nv}$, then all the described invariants vanish. This situation describes $C_{4v}$ and $C_{6v}$, and is proven in Sec. 3.7.1 below. In $C_{3v}$ systems, the only consequence of (3.61) is that $\chi_1 = \chi_3$ for $C_{3v}^{(b)}$, as shown in Sec. 3.7.2.
3.7.1 Vanishing invariants of $C_{4v}$ and $C_{6v}$

If the BdG energy spectrum is gapped at momentum $k$, we may define the Berry vector potential as

$$\mathcal{A}(k) = -i \sum_{E_n < 0} \langle u_{n,k} | \nabla | u_{n,k} \rangle,$$

(3.62)

for $|u_{n,k}\rangle$ an eigenstate of the BdG Hamiltonian $H(k)$. Here we sum over all bands with negative energies. The negative-energy Berry field is defined as

$$\tilde{F}(k) = \nabla \times \mathcal{A}(k).$$

(3.63)

Analogously, it is convenient to define a positive-energy Berry field:

$$\tilde{G}(k) = -i \sum_{E_n > 0} \nabla \times \langle u_{n,k} | \nabla | u_{n,k} \rangle.$$  

(3.64)

The particle-hole transformation of (3.61) relates a positive-energy state at $k$ to a negative-energy state at $-k$; the negative-energy and positive-energy Berry fields are thus related by

$$\tilde{F}(k) = -\tilde{G}(-k).$$

(3.65)

A useful relation is that the Berry field of all bands is zero, i.e.,

$$\tilde{F}(k) + \tilde{G}(k) = 0,$$

(3.66)

if the superconductor is gapped at $k$. The proof consists of considering an infinitesimal Wilson loop $W[l]$ around an area element $d\Omega$, centered at momentum $\tilde{k}$. From Stoke’s theorem,

$$\exp\left[ i (\tilde{F}(\tilde{k}) + \tilde{G}(\tilde{k})) \cdot d\Omega \right] = \det W[l],$$

(3.67)

and the discretized Wilson loop has the form

$$W[l]_{ij} = \langle u_{\tilde{k},i} | \prod_{q \in l} P_{alt}(q) | u_{\tilde{k},j} \rangle,$$

(3.68)
where the product of projections are path-ordered around the perimeter \( l \) of \( d\Omega \). Since \( P_{\text{all}} \) is the projection onto all bands, by the completeness property it is just the identity. Thus,

\[
( \tilde{F}(\tilde{k}) + \tilde{G}(\tilde{k}) ) \cdot d\Omega = 2\pi u; \quad u \in \mathbb{Z}.
\]  

(3.69)

\( \tilde{F} \) and \( \tilde{G} \) are bounded if there is no singularity due to a band-touching at \( \tilde{k} \). Since \( d\Omega \) is infinitesimal, and \( \tilde{F} + \tilde{G} \) bounded, \( u = 0 \). Since this proof works for any orientation of the area element, and for any \( \tilde{k} \) where the superconductor is gapped, we have proven (3.66).

Combining (3.65) with (3.66),

\[
\tilde{F}(k) = \tilde{F}(-k).
\]  

(3.70)

Now consider a momentum \( k \) in a mirror plane (MP) of a \( C_{4v} \) or \( C_{6v} \) system. All Bloch wavefunctions in MP may be diagonalized by a single operator, which represents the reflection \( M_i \). Since the particle-hole transformation commutes with \( M_i \), (3.70) implies \( \mathcal{F}_e(k) = \mathcal{F}_e(-k) \), where \( \mathcal{F}_e \) is the component of \( \tilde{F}_e \) perpendicular to MP. Suppose there exists a two-fold rotational symmetry \( C_2 \), with axis parallel to the principal \( C_n \) axis. For spinless representations, \( M_i C_2 M_i^{-1} = C_2^{-1} = C_2 \), thus their operations commute. This implies that a mirror-even state at momentum \( k \) is related by two-fold symmetry to a mirror-even state at \( D(C_2)k \), where \( D(C_2) \) is the representation of the two-fold rotation in \( \mathbb{R}^3 \). This implies \( \mathcal{F}_e(k) = -\mathcal{F}_e(-D(C_2)k) \). By the same argument we deduce that \( \mathcal{F}_e(t_i, k_z) = -\mathcal{F}_e(t_i, -k_z) \), for a momentum \((t_i, k_z)\) in a half-mirror-plane (HMP\(_i\)), and similarly \( \mathcal{F}_o(t_i, k_z) = -\mathcal{F}_o(t_i, -k_z) \) for the odd subspace. This implies \( B_e^{(i)} = B_o^{(i)} = 0 \), as defined in (3.50). Then the halved chirality is zero because \( 2\pi \chi_i = B_e^{(i)} - B_o^{(i)} = 0 \). By similar arguments, we may derive that the mirror Chern numbers and the bent Chern numbers vanish.

### 3.7.2 \( \chi_1 = \chi_3 \) in spinless \( C_{3v}^{(b)} \) superconductors

We refer to Fig. 3.7(b). A product of particle-hole transformation and a three-fold rotation relates states in HMP\(_1\) to states in HMP\(_3\), thus \( B_e^{(1)} = B_e^{(3)} \), and \( B_o^{(1)} = B_o^{(3)} \). This implies...
$\chi_1 = \chi_3$. There are no constraints on the other invariants of $C_{30}^{(b)}$. 
Chapter 4

Hourglass Dirac fermions and the Crystalline Spin Hall Effect

The previous Chapter introduced a symmorphic band topology which manifests both in the bulk and the surface. Here, we show that non-symmorphic symmetries result in new band topologies that have no symmorphic analog, as well as propose KHgX (X = As, Sb and Bi) as the first material realization of a non-symmorphic topology. The topology of KHgX manifests differently on its various surfaces, depending on the spatial symmetries which are preserved on that surface. On the 010 surface, we find that the glide-mirror symmetry protects a novel surface Dirac fermion that is shaped like an hourglass (see Fig. 4.1(d)); doubly-degenerate surface bands connect one hourglass to the next in a zigzag pattern that robustly interpolates across the conduction gap in Fig. 4.1(a). In constrast, the 100 surface uniquely realizes a 3D doubled quantum spin hall effect (QSHE) with four counter-propagating surface modes distinguished by spin, as illustrated in Fig. 4.1(f). Unlike the well-known 2D QSHE (Fig. 4.1(e)), our surface states are not protected by time-reversal symmetry alone, but are instead stabilized by spatial symmetries. To describe the bulk topology of KHgX, we will introduce a non-Abelian generalization of polarization that naturally describes crystals with glide-mirror symmetry, and is moreover quantized in the presence of spatial inversion symmetry; our work is thus an extension of the well-known
Abelian theory of polarization. [47–49] Finally, our material class uniquely exemplifies an inversion of its rotational quantum numbers, which we propose as a fruitful criterion in the search for topological materials.

Figure 4.1: (a–c) Examples of the possible topologies of surface bands in a non-symmorphic crystal. All crossings along \( \tilde{\Gamma}\tilde{X}\tilde{U} \) and degeneracies along \( \tilde{U}\tilde{Z} \) arise from symmetry. (a) corresponds to our material class, (b) to the trivial topology, and (c) to a nontrivial topology which may be found in other materials. (d) Hourglass-shaped Dirac fermion in KHgSb. (e) The well-known 2D quantum spin Hall effect, with a pair of spin-split modes counter-propagating on the edge. (f) Crystalline spin Hall effect in a nutshell: two right-going surface modes with spin up, and two left-going modes with spin down. These surface modes are protected by a reflection symmetry that is indicated by parallel diagonal lines.

The crystal structure of KHgX is illustrated in Fig. 4.2: the Hg and X ions form honeycomb layers with AB stacking along \( \tilde{z} \); between each AB bilayer sits a triangular lattice of K ions. The spatial symmetries include: (i) an inversion \( (I) \) centered around a K ion, which we henceforth take as our spatial origin, (ii) the screw rotation \( \bar{C}_{6z} \) is a six-fold rotation about \( \tilde{z} \) followed by a fractional lattice translation \( (t(c\tilde{z}/2)) \). Here and henceforth, for any transformation \( g \), we denote \( \bar{g}=t(c\tilde{z}/2)g \) as a product of \( g \) with this fractional translation. (iii) Finally, we have the reflections \( M_y : (x,y,z)\rightarrow(x,-y,z) \), \( \bar{M}_z=t(c\tilde{z}/2)M_z \) and \( \bar{M}_x \). Among these only \( \bar{M}_x \) is a glide reflection, wherefor the fractional translation is unremovable by a different choice of origin. Altogether, these symmetries generate the non-symmorphic space group \( D^{1}_{6h}(P6_3/mmc) \). The topological features of KHgX may
each be attributed to a subset of these symmetries, rather than the entire group – on surfaces where certain bulk symmetries are lost, their associated topology is not manifest.

We will find that the 100-surface symmetry is a symmorphic subgroup of $D_{6h}$, leading to strikingly different bandstructure from the non-symmorphic 010 surface. Our strategy is to first deduce the possible topologies of the surface bands purely from representations of the surface symmetry. We then more carefully account for the bulk symmetries and the orbital character of our bands, as well as introduce a non-Abelian polarization that characterizes the bulk wavefunctions.

Let us first discuss the 010 surface, whose symmetry group ($P_{ma2}$) is generated by glideless $\bar{M}_z$ and glide $\bar{M}_x$. To explain the robust surface bands in Fig. 4.1, we consider each high-symmetry line in turn: (i) At any wavevector ($k'$) along the line $\bar{Z}\bar{U}$ ($k_z=\pi/c$), all bands are doubly degenerate. Indeed, the group [18] of $k'$ includes the antiunitary element $T\bar{M}_x$ (which combines time-reversal with a glide), whose non-symmorphic representation squares to the negative identity, resulting in a Kramers-like degeneracy at each $k'$. (ii) The two glide-invariant lines are $\bar{Γ}\bar{Z}$ (parametrized by $(k_x=0, k_z)$) and $\bar{X}\bar{U}$ (by $(k_x=\pi/\sqrt{3}a, k_z)$). Along both lines, bands split into quadruplets which each exhibits an internal partner-switching in the interval $k_z \in [0, \pi/c]$. To explain this internal partner-switching, first recall

![Figure 4.2: (a) 3D view of atomic structure. The Hg (red) and X (blue) ions form a honeycomb layers with AB stacking. The K ion (cyan) is located at an inversion center, which we also choose to be our spatial origin. (b) Top-down view of a truncated lattice with two surfaces. (c) Center: bulk Brillouin zone (BZ) of KHgX, with two mirror planes of $\bar{M}_z$ colored red and blue. Top: 100-surface BZ. Right: 010-surface BZ.](image-url)
that the glide squares as $\tilde{M}_x^2 = t(c\bar{z}) \bar{E}$, with $\bar{E}$ denoting a $2\pi$ rotation and $t$ a lattice translation. Equivalently, the Bloch-wave representation of $\tilde{M}_x$ squares to $-\exp(-ik_z/c)$, which implies two branches for the mirror eigenvalues: $\pm i\exp(-ik_zc/2)$. The role of time-reversal symmetry is to enforce degeneracies between complex-conjugate representations of $\bar{M}_x$ at both Kramers points, i.e., $[T, \bar{M}_x] = 0$ leads to a pairing of the $\bar{M}_x$ eigenvalues as $\{+i, -i\}$ at $k_z = 0$, and either $\{+1, +1\}$ or $\{-1, -1\}$ at $k_z = \pi/c$. Given these constraints, there are two topologically distinct connectivities for the surface bands. The first is illustrated in Fig. 4.3(c): surface bands zigzag across the conduction gap and each cusp is a Kramers doublet – this may be viewed as a glide-symmetric analog of the 2D QSHE, as will be elaborated. The second connectivity in Fig. 4.3(d) applies to our material class: an internal partner-switching occurs within each quadruplet, resulting in an hourglass-shaped dispersion. The center of each hourglass is a robust crossing between orthogonal mirror branches – we thus have an unpinned Dirac fermion in the interval $k_z \in [0, \pi/c]$, as further exemplified by KHgSb in Fig. 4.1(d). Henceforth, we choose KHgSb to represent KHgX, which all exhibit the same topology. To recapitulate, the surface bands form doubly-degenerate doublets along $\tilde{Z}\tilde{U}$, and hourglasses along $\tilde{\Gamma}\tilde{Z}$ and $\tilde{X}\tilde{U}$; when viewed individually on each line, neither case interpolates across the conduction gap. However, when viewed collectively along a bent line ($\tilde{X}\tilde{U}\tilde{Z}\tilde{\Gamma}$), the possibility of a robust interpolation arises. At $\tilde{Z}$ and $\tilde{U}$, there are two ways to connect hourglasses to degenerate doublets: the first is the zigzag connectivity drawn in the $\tilde{X}\tilde{U}\tilde{Z}\tilde{\Gamma}$ section of Fig. 4.1(a), which is equivalent to the surface bands of KHgSb (in Fig. 4.3(a)) with an ideal surface termination. By ‘equivalent’, we mean that the surface-localized bands also connect with the surface-resonant bulk bands in this hourglass-zigzag topology. To confirm this equivalence, we modified the surface potential of KHgSb to push the hourglass (along $\tilde{\Gamma}\tilde{Z}$) down into the valence band; due to the proposed hourglass-zigzag, a different hourglass is pulled down from the conduction band along $\tilde{U}\tilde{X}$ (see Fig. 4.3(b)). Our hourglass-zigzag is distinguished from a second possible connectivity without robust surface states (see $\tilde{X}\tilde{Z}\tilde{U}\tilde{\Gamma}$ section of Fig. 4.1(b)). Finally, we turn to the last high-symmetry line: (iii) along $\tilde{\Gamma}\tilde{X}$ ($k_z = 0$), bands divide into two subspaces having
either $\bar{M}_z$-eigenvalue $+i$ or $-i$, as follows from $M_z^2 = \bar{E}$. The two chiral (anti-chiral) surface modes in the $+i$ (resp. $-i$) subspace may be summarized by a mirror Chern number [34] $C_e = +2$.

![Figure 4.3](image)

Figure 4.3: The 010-surface bands of KHgSb for an ideal surface termination in (a), and with a modified surface potential in (b). (c-d) Possible surface topologies along $\bar{\Gamma}\bar{Z}\bar{Z}$. Solid and dashed distinguish between two eigenvalue branches of $\bar{M}_z$: $\pm i \exp(-ik_z c/2)$.

Since the 100 surface also preserves the glideless $\bar{M}_z$, the 100 dispersion along $k_z = 0$ ($\bar{\Gamma}\bar{Y}$ in Fig. 4.4(a)) is topologically equivalent to that of the 010 along $\bar{\Gamma}\bar{X}$ – this reflects two distinct surface projections of the same bulk topology, as we illustrate in Fig. 4.2(c). One begins to see striking differences away from $\bar{\Gamma}\bar{Y}$: the 100 surface modes barely disperse with $k_z$, forming the anisotropic band structure in Fig. 4.4(c); the spin structure at the Fermi level is revealed in Fig. 4.4(b). At low energies, we then realize a 3D doubled QSHE, with two sets of right-moving, spin-down carriers and their time-reversed partners.

![Figure 4.4](image)

Figure 4.4: (a) The 100-surface bandstructure over a momentum rectangle. While a small hybridization gap ($\sim 1$ meV) opens for $k_z \neq 0$, along $k_z = 0$ is a robust intersection between $\bar{M}_z = \pm i$ subspaces. (b) Spin texture at the Fermi level.

Having enumerated the possible surface topologies purely from consideration of the
Figure 4.5: (a) The bulk bandstructure of KHgSb. The size of each red dot quantifies the weight of Hg-\(s\) orbitals. (b-c) Orbital character of KZnP (top) and KHgSb (bottom) at any point along \(\Gamma A\), as we vary the crystal field and spin-orbit coupling from zero (leftmost) to their natural strengths (rightmost). The precise wavefunctions of \(S_{1/2}\), \(P_{3/2}\), \(P_+\) and \(P_-\) are clarified in the Supplementary.

surface symmetries, we now identify which of these topologies are consistent with the bulk symmetries, with emphasis on the particular symmetry representations in KHg\(X\). Our first-principles calculation of KHgSb show that the relevant orbitals near the Fermi energy comprise one \(s\)-type quadruplet (derived from Hg) and three \(p\)-type quadruplets (from Sb); a bulk gap of approximately 0.2 eV is induced by spin-orbit splitting of the \(p\)-type bands. Given that electrons fill 12 of these 16 bands, two scenarios emerge: (i) If only the \(p\)-type bands are occupied, as exemplified by KZnP in Fig. 4.5(b), then the lack of hybridization between Zn and P suggests a trivial insulating phase. (ii) With KHgSb, the occupied bands along \(\Gamma A\) have mixed \(s\)- and \(p\)-character (Fig. 4.5(c)), which suggests that its Wannier functions localize between the Hg and Sb atoms – since the 010-surface termination also occurs between atoms, these off-atom Wannier functions mutually hybridize to form surface states. To precisely formulate this intuition, we employ a Bloch-Wannier (BW) representation [50] of the occupied bands: given \(n_{occ}\) occupied bands, we can represent them as a set of hybrid functions \(\{|\mathbf{k}_n, n\rangle | n \in \{1, 2, \ldots, n_{occ}\}\}\) which maximally localize in \(\bar{y}\) (as a Wannier function) but extend in \(\bar{x}\) and \(\bar{z}\) (as a Bloch wave with momentum \(\mathbf{k}_n=(k_x, k_z)\)). Each BW function is constructed to be an eigenfunction of the projected position operator \(P\hat{y}P\), where \(P\) denotes the projection to the occupied bands; the eigenvalue \((y_{n,\mathbf{k}_n})\) under \(P\hat{y}P\) is merely the center-of-mass coordinate of the BW function \(|n, \mathbf{k}_n\rangle\). [51] Due to the discrete translational symmetry of \(P\), each \(y_{n,\mathbf{k}_n}\) is a mod-integer quantity that represents
a family of eigenfunctions related by integer translations – here, $1 \equiv a/2$ is the translational period in $\tilde{y}$. Given that the spectrum of $P\hat{y}P$ can be interpolated [52, 53] to the 010-surface bandstructure (Fig. 4.3(a)) while preserving the 010 symmetries, we expect [50] that both spectra share similar features. These features may be found in Fig. 4.6, and include: (i) degenerate doublets along $\tilde{Z}\tilde{U}$, (ii) partner-switching quadruplets along $\tilde{\Gamma}\tilde{Z}$ and $\tilde{X}\tilde{U}$, and (iii) robust crossings between orthogonal $\tilde{M}_z$ subspaces along $\tilde{\Gamma}\tilde{X}$. However, differences arise because the spectrum of $P\hat{y}P$ additionally encodes bulk symmetries which are spoiled by the 010 surface. One difference lies in the possibility of a glide-symmetric QSHE outside our material class: while our naive surface argument allows for a zigzag connectivity (Fig. 4.3(c)) along both $\tilde{\Gamma}\tilde{Z}$ and $\tilde{X}\tilde{U}$, the out-of-surface translational symmetry rules out this scenario along $\tilde{X}\tilde{U}$. A second difference originates from the bulk inversion ($I$) symmetry, which quantizes two invariants that have no surface analog; as will be clarified, these invariants describe a coarse-grained polarization of quadruplets along the glide lines $\tilde{\Gamma}\tilde{Z}$ and $\tilde{X}\tilde{U}$. For illustration, we consider the top quadruplet along $\tilde{X}\tilde{U}$, which is magnified in Fig. 4.6(b) – the center-of-mass position of this quadruplet may tentatively be defined by averaging four BW positions: $Y_1(k_q) = (1/4)\sum_{n=1}^{N} y_{n,k_q}$. We caution that $Y$ is ill-defined (mod one) at any generic $k_q$, due to the aforementioned integer ambiguity of $\{y\}$. The following discussion hinges on the connectivity of the quadruplet along $\tilde{X}\tilde{U}$, i.e., that there are enough contact points along $\tilde{X}\tilde{U}$ to continuously travel between the four branches of $\{y_{n,k_q}\}_{n=1,2,3,4}$. Indeed, supposing we fix $y_1 \approx 0.22$ in Fig. 4.6(b) (e.g., instead of 1.22 or $-0.78$), then $y_2$, $y_3$ and $y_4$ are uniquely determined as the branches that connect to $y_1$ – clearly then $Y_1(k_q) \approx 0.22$ as well, and more generally $Y_1$ is well-defined mod one. Having defined a center-of-mass coordinate for one quadruplet, we extend our discussion to the net displacement of all $n_{occ}/4$ number of quadruplet centers: $Q(k_{oc})/e = \sum_{j=1}^{n_{occ}/4} Y_j(k_{oc}) \mod 1$. A combination of time-reversal ($T$) and spatial-inversion ($I$) symmetry quantizes $Q(k_{oc})$ to 0 or $e/2$, as we now show. Consider how $TI$ inverts the spatial coordinate but leaves momentum untouched, i.e., we have a ‘particle-hole’ symmetry at each $k_{oc}$: $TI|k_{oc},n\rangle = |k_{oc},m\rangle$ with $m \neq n$ and $y_{n,k_{oc}} = -y_{m,k_{oc}} \mod 1$. Consequently, $TI : Y_j(k_{oc}) \rightarrow Y_j(k_{oc}) = -Y_j(k_{oc}) \mod 1$, and the
only non-integer contribution to $Q/e$ arises from a particle-hole-invariant quadruplet ($\bar{j}$) that is centered at $\bar{Y}_j=1/2=-\bar{Y}_j \mod 1$. This quantization ensures a constant value of $Q$ along each glide line – we therefore have two $\mathbb{Z}_2$ invariants: $Q_{\bar{t}2}$ and $Q_{\bar{X}0}$. For KHgSb, inspection of Fig. 4.6 leads to $Q_{\bar{X}0}=0$ and $Q_{\bar{t}2}=e/2$ – this difference originates from the band inversion along $\Gamma A$ (cf. Fig. 4.5). Wherever $Q_{\bar{t}2} \neq Q_{\bar{X}0}$, the degenerate doublets along $\bar{Z}\bar{U}$ must connect the ‘upper handle’ of an hourglass at $\bar{Z}$, to a ‘lower handle’ at $\bar{U}$, as illustrated in Fig. 4.6(a); for comparison, Fig. 4.6(e) depicts the trivial spectrum for KZnP.

To return to our original motivation, $Q_{\bar{t}2}=e/2$ in KHgSb precisely indicates the desired off-atom Wannier center; due to a 010 surface termination, these off-atom BW functions hybridize to form the surface hourglass of Fig. 4.3(a).

Figure 4.6: (a) Spectrum of $P\hat{y}P$ for KHgSb. (b-d) Close-ups of (a). (f) Spectrum of $P\hat{y}P$ for KZnP, with corresponding close-up (e).

Beside having different quadruplet polarizations, KHgSb and KZnP are further distinguished by their quantum numbers under spatial transformations; we will connect these quantum numbers to the mirror Chern number in the $k_z=0$ plane. By far the most successful strategy [54] in finding topological materials lies in identifying centrosymmetric systems with inverted parity quantum numbers. [7,34,35,39,55–57] For KHgSb, the parity eigenvalues of the $s$-quadruplet (recall Fig. 4.5) are identical with those of any $p$-quadruplet, and therefore there is no parity inversion at any inversion-invariant momentum. Following the well-known parity criterion, previous works have thus concluded that KHgSb is topologically trivial. [58,59] Instead, our material class is distinguished by having an inversion of
its rotational eigenvalues, which we propose as a new criterion in the search for topological materials. Specifically, we consider the eigenvalues \( \exp[-i\pi J_z/3] \) of these two quadruplets under the screw rotation \( \bar{C}_{6z} \). Since \([\bar{C}_{6z}, \bar{M}_z]=0\), states at \( \Gamma \) can simultaneously be labeled by both operators. The \( \bar{M}_z=+i \) states in the \( s \)-quadruplet (\( p \)-quadruplet) transform as \( J_z=-1/2 \) and \( 5/2 \) (resp. \( J_z=3/2 \) and \( -3/2 \)), and their inversion at \( \Gamma \) results in a net angular momentum gain of \( \Delta J_z=2 \), which accompanies a quantized redistribution of Berry curvature, \([27]\) i.e., \( \Delta J_z \) is equal to the change in the mirror Chern number \( (C_e) \) modulo six. We confirm that \( C_e=2 \) using the method of Wilson loops, in further accordance with our surface analysis.

The rest of the Chapter supplements our main results. In Sec. 4.1, we elaborate on the diagnosis of topological invariants from bulk wavefunctions. Through the Wilson loop, we propose an efficient method to diagnose mirror Chern numbers in time-reversal-invariant systems, and apply our method to our material class. We also prove that some topologies cannot exist on certain mirror planes. Sec. 4.2 outlines a general strategy to find topological materials which are rotationally inverted, as well as provides a detailed case study for our material class. We conclude with a few remarks in Sec. 4.3.

### 4.1 Diagnosing bulk topological invariants

Our aim is to diagnose topological invariants from bulk wavefunctions. As described in the main text, one useful diagnosis tool is the spectrum of the projected-position operator \( (P\hat{y}P) \). Sec. 4.1.1 reveals the easiest way to calculate this spectrum – by relating \( P\hat{y}P \) to a Wilson loop, which also demonstrates an instructive connection with holonomy. Building upon this, we then propose an efficient way to extract the mirror Chern number in crystals with time-reversal symmetry, and as a case study, we applied our method to the \( k_z=0 \) mirror plane of KHgSb in Sec. 4.1.2. In contrast, the mirror Chern number in the \( k_z=\pi/c \) plane must vanish for our space group, as we demonstrate in Sec. 4.1.3. Finally in Sec. 4.1.4, we argue that there can be no quantum spin Hall effect in the \( k_x=\pi/\sqrt{3}a \) glide plane.
4.1.1 Review of Wilson loops and the projected-position operator

Figure 4.7: (a) A constant-\(k_z\) slice of quasimomentum space, with two of three reciprocal lattice vectors indicated by \(\tilde{b}_1\) and \(\tilde{b}_2\). While each hexagon corresponds to a Wigner-Seitz primitive cell, it is convenient to pick the rectangular primitive cell that is shaded in cyan. A close-up of this cell is shown in (b). Here, we illustrate how the glide reflection \((\tilde{M}_x)\) maps \((k_y, \pi/\sqrt{3} a, k_z) \rightarrow (-k_y, -\pi/\sqrt{3} a, k_z)\) (red dot to brown) which connects to \((2\pi/a + k_y, \pi/\sqrt{3} a, k_z)\) (blue) through \(\tilde{b}_2\). Figure (c) serves two interpretation. In the first, \(TM_z\) maps \((k_y, \pi/\sqrt{3} a, k_z) \rightarrow (-k_y, -\pi/\sqrt{3} a, k_z)\) (red dot to brown) which connects to \((2\pi/a - k_y, \pi/\sqrt{3} a, k_z)\) (blue) through \(\tilde{b}_2\). If we interpret Figure (c) as the \(k_z = 0\) cross-section, the same vectors illustrate the effect of time reversal.

The spectrum of the projected-position operator \((P\tilde{y}P)\) is obtained by diagonalizing a Wilson-loop operator, which effects parallel transport of the occupied bands along a non-contractible loops in the BZ. We consider a family of loops parametrized by \(k_{ni} = (k_x, k_z) \in [-\pi/\sqrt{3} a, +\pi/\sqrt{3} a], k_z \in [-\pi/c, +\pi/c]\), where for each loop \(k_{ni}\) is fixed while \(k_y\) is varied over a non-contractible circle (colored red in Fig. 4.7(a)). In the orbital basis, such transport is represented by the Wilson-loop operator

\[
W(k_{ni}) = V(4\pi \tilde{y} / a) \prod_{k_y}^{2\pi/a\leftarrow -2\pi/a} P(k_y, k_{ni}), \tag{4.1}
\]

where we have discretized the momentum as \(k_y = 4\pi m/(aN_y)\) for integer \(m = 1, \ldots, N_y\), and \((2\pi/a \leftarrow -2\pi/a)\) indicates that the product of projections is path-ordered. Here \(a/2\) is the lattice period in \(\tilde{y}\), and \(4\pi \tilde{y} / a\) is a reciprocal lattice vector. In the limit of large \(N_y\), the eigenvalues of \(W\) become unimodular, and we label them by \(\exp[i\theta_{n,k_{ni}}]\) with \(n = 1, \ldots, n_{occ}\).

Denoting the eigenvalues of \(P\tilde{y}P\) as \(y_{n,k_{ni}}\), the two spectra are related as \(y_{n,k_{ni}} = \theta_{n,k_{ni}} / 2\pi\) modulo one. [51]
4.1.2 Mirror Chern number in the \( k_z = 0 \) mirror plane

For time-reversal-invariant crystals, we propose an efficient method to calculate the mirror Chern number \( (C_e) \) by non-Abelian Berry phases – by exploiting the time-reversal symmetry, we are able to extract \( C_e \) from wavefunctions in half of a mirror plane.

Our topological invariant is defined as the integrated Berry flux [27] through the \( k_z = 0 \) mirror plane, as contributed by the even \( (M_z = +i) \) subspace of reflection:

\[
C_e = \frac{1}{2\pi} \int_0^{2\pi} dk_x \int_0^{2\pi} dk_y F_e(k_x, k_y). \tag{4.2}
\]

We emphasize that \( M_z \) is not a glide reflection, so we may choose a spatial origin which is preserved by this symmetry, e.g., the center in the plane of a hexagon in Fig. 4.2. In spin-orbit-coupled systems, time-reversal symmetry relates even and odd \( (M_z = -i) \) subspaces by \( F_e(k_x, k_y) = -F_o(-k_x, -k_y) \), and therefore we re-express

\[
C_e = \frac{1}{2\pi} \int_0^{\pi} dk_x \int_0^{2\pi} dk_y (F_e(k_x, k_y) - F_o(k_x, k_y)) \tag{4.3}
\]

as an integral over half of a mirror plane. By Stoke’s theorem, we may relate an integral of curvature to differences in the Wilson-loop phases \( \{\theta\} \). [51] Due to the orthogonality of the mirror subspaces, we may label each \( \theta \)-band by its mirror eigenvalue: \( \theta^e (\theta^o) \) in the even (odd) subspace is colored red (blue) in Fig. 4.8. \( C_e \) is thus further rewritten as the net change in \( \theta^o \) in the interval \( k_x \in [0, \pi] \), minus the net change in \( \theta^e \):

\[
C_e = \frac{1}{2\pi} \int_0^{\pi} dk_x \sum_{i=1}^{n_{occ}/2} \left( \frac{\partial \theta^o_i}{\partial k_x} - \frac{\partial \theta^e_i}{\partial k_x} \right). \tag{4.4}
\]

Here, we have distinguished different Wilson-loop phases by a band index in the subscript of \( \theta \); given \( n_{occ} \) occupied bands, time-reversal symmetry ensures an even split between even and odd representations. \( C_e \) is most easily extracted from \( \{\theta\} \) by a ‘Fermi-level’ criterion: consider the intersections of \( \{\theta\} \) with an arbitrary constant-phase line. At each intersection, we evaluate \( \text{[sign of } \partial \theta / \partial k_x \text{] \times [mirror eigenvalue/i]} \), then sum this quantity over all intersections along \( k_x \in [0, \pi] \). Applying this method to Fig. 4.8, we find \( C_e = 2 \) for KHgSb.
Figure 4.8: (a) Wilson-loop spectrum along $\tilde{\Gamma} \tilde{Z}$. (b) is a close-up of (a).

We briefly remark that time-reversal symmetry in spinless systems instead relates $F_e(k_x, k_y) = -F_e(-k_x, -k_y)$ which causes $C_e$ to vanish. Nevertheless, the right-hand side of Eq. (4.3) is independently valid as a different topological invariant, which we have shown to be quantized in rotationally-symmetric crystals. [60]

4.1.3 Vanishing of mirror Chern number in the $k_z = \pi/c$ plane

Given that the rotational inversion along $\Gamma - A$ leads to nontrivial band topology in the $k_z = 0$ plane, we might ask if the $k_z = \pi/c$ mirror plane manifests the same topology. We find for the latter plane that spin-degenerate partners belong in the same $\bar{M}_z$ subspace, thus contributing canceling Berry curvatures at each momentum; in contrast, spin-degenerate partners in the $k_z = 0$ plane belong in opposite mirror subspaces. This is more generally true for any space group with inversion and glideless-mirror symmetries that preserve different origins, i.e., $\bar{M}_z I = t(c\vec{z}) I \bar{M}_z$.

Proof At each wavevector ($\tilde{k}$) in this mirror plane, the mirror-projected Berry curvatures must vanish, i.e., $F_e(k) = F_o(k) = 0$, as we now demonstrate. The group of $\tilde{k}$ comprises $TL$ and $\bar{M}_z$, whose representations anticommute due to two reasons: (i) From $\bar{M}_z L = t(c\vec{z}) L \bar{M}_z$, the translation ($t$) acts on a Bloch wave to produce a phase factor ($\exp[-ik_z c]$) which equals $-1$ presently. (ii) Being spatially local, time reversal commutes with any space group element. It follows that if $|\psi(\tilde{k})\rangle$ is an eigenstate of $\bar{M}_z$, its spin-degenerate partner ($TL|\psi(\tilde{k})\rangle$) belongs in the same mirror subspace. Since $TL$ is antiunitary, spin-degenerate
partners contribute canceling Berry curvatures, thus ruling out a quantum anomalous Hall effect within the same mirror subspace.

4.1.4 No QSHE in the \( k_x = \pi/\sqrt{3}a \) glide plane

The \( k_x = \pi/\sqrt{3}a \) plane is invariant under both glide-reflection and time-reversal symmetries. In the first step, we formulate a QSH topology in this plane by assuming only time-reversal symmetry, and then we show the effect of glide symmetry is to rule out the QSH phase altogether.

The time-reversal-invariant momenta in this glide plane lie at

\[
(k_y, k_z) \in \{ (\pm \pi/a, 0), (\pm \pi/a, \pi/c) \},
\]

as follows from time reversal mapping \( \mathbf{k} = (\pi/\sqrt{3}a, k_y, k_z) \rightarrow -\mathbf{k} \), which further connects to \((\pi/\sqrt{3}a, 2\pi/a - k_y, -k_z)\) through a reciprocal vector illustrated in Fig. 4.7(c). We follow the Kane-Mele formulation [3] of the \( Z_2 \) invariant by defining the skew-symmetric matrix

\[
[A_k]_{ij} = \langle u_i, k | \hat{T} | u_j, k \rangle K, \quad \text{with} \quad i, j = 1, \ldots, n_{occ},
\]

and its Pfaffian by \( \zeta_k = \text{Pf}[A_k] \); here, we have represented time reversal by the anti-unitary operator \( \hat{T} = U_T K \). The Kane-Mele criterion for a QSH phase is an odd number of zeros of \( \zeta \) in half the glide plane, [3] which implies at least one of these zeros can never be annihilated, e.g., see Fig. 4.9(a). To be concrete, we take the half-glide plane with \( k_z \in [0, \pi/c] \). To simplify our argument, we have assumed the zeros of \( \zeta \) form isolated points instead of lines, as would be the case without spatial-inversion symmetry. Now we show that the presence of the glide-mirror symmetry ensures that zeros, if they exist, can always mutually annihilate.

**Proof** Consider the glide reflection \( M_x \), which transforms spatial coordinates as \((x, y, z) \rightarrow (-x, y, z + 1/2)\). In the glide plane, \( M_x \) maps between two momenta which are separated by half a reciprocal period: \((k_y, \pi/\sqrt{3}a, k_z) \rightarrow (k_y, -\pi/\sqrt{3}a, k_z) = (k_y + 2\pi/a, \pi/\sqrt{3}a, k_z) - \hat{b}_2\),
\begin{align*}
\left|u_{m,k_y+2\pi/a}\right> &= e^{-ik_zc/2} \sum_{n=1}^{n_{occ}} [\tilde{U}_{k_y+2\pi/a-e-k_y}]^*_{mn} V(-\tilde{b}_2) U_{\delta x} |u_{n,k_y}\rangle, \quad (4.7)
\end{align*}

where exp\((-ik_zc/2)U_{\delta x}\) represents \(M_x\) in the Bloch-orbital basis, \(\tilde{U}\) is a unitary matrix and we suppress the common label \(k_x\). Combining this glide constraint with Eq. (4.8),

\begin{align*}
[A_{k_y+2\pi/a}]_{ij} &= \sum_{\alpha,\beta=1}^{n_{tot}} u_{i,k_y+2\pi/a}(\alpha)\ast [U_T]_{\alpha\beta} u_{j,k_y+2\pi/a}(\beta)\ast \\
&= e^{ik_zc} \sum_{\mu,\nu=1}^{n_{tot}} \sum_{m,n=1}^{n_{occ}} [\tilde{U}_{k_y+2\pi/a-e-k_y}] \text{im} \ u_{m,k_y}(\mu)\ast \left[U_{\delta x}^\dagger V(\tilde{b}_2) U_T V(\tilde{b}_2) U_{\delta x}^*\right] \mu\nu \ u_{n,k_y}(\nu)\ast [\tilde{U}_{k_y+2\pi/a-e-k_y}]_{nj}.
\end{align*}

(4.8)

Two more identities are useful: (i) since time reversal commutes with spatial transformations, \(U_T U_{\delta x}^* = U_{\delta x} U_T\), and (ii) \(U_T V(\tilde{b}_2) = V(-\tilde{b}_2) U_T\) follows from identifying \(D_g = I\) and \(\delta = 0\) in Eq. (1.38). Combining these identities with Eq. (4.8), we are led to

\begin{align*}
A_{k_y+2\pi/a} &= e^{ik_zc} \tilde{U}_{k_y+2\pi/a-e-k_y} A_{k_y} \tilde{U}_{k_y+2\pi/a-e-k_y}^t.
\end{align*}

(4.9)

Applying a well-known Pfaffian identity, we conclude that

\begin{align*}
\zeta_{k_y+2\pi/a,k_x} &= e^{in_{occ}k_zc} \text{det}(\tilde{U}_{k_y+2\pi/a-e-k_y}) \zeta_{k_y,k_x}.
\end{align*}

(4.10)
Since (i) $\bar{U}$ is unitary, and (ii) both $\exp(i n_{oc} k_z c)$ and $\bar{U}$ are analytic functions of $k$, zeros of $\zeta$ always appear as glide-related pairs of the same vorticity, which we define by the phase-winding of $\zeta$ around each zero. Each glide-related pair belongs to the same half-glide plane; recall here that the two half planes are defined by $k_z \in [0, \pi/c]$ and $k_z \in [-\pi/c, 0]$. Due to time-reversal symmetry, every glide-related pair in one half plane has a partner pair in the other half plane with opposite vorticity, as we illustrate in Fig. 4.9(b). The same figure demonstrates this minimal set of zeros can always mutually annihilate.

4.2 Searching for rotationally-inverted topological insulators

To efficiently diagnose topological materials, we propose to search for inversions of the rotational quantum numbers. Such a criterion to diagnose the quantum anomalous Hall effect (QAHE) is already known [61] for symmorphic space groups, and in Sec. 4.2.1 we generalize this criterion to describe any space group. In Sec. 4.2.2, we describe how rotational inversion can lead to a nontrivial mirror Chern number, as we exemplify with the KHgX material class.

4.2.1 Quantum anomalous Hall effect due to rotational inversion

Let us consider a space group with an $\bar{n}$-fold rotational symmetry ($C_{\bar{n}, \delta}$); our discussion applies to both screw ($\delta \neq 0$) and normal ($\delta = 0$) rotations, as well as to integer- and half-integer-spin representations. If nonzero, $\delta$ always lies parallel to the rotational axis, [6] which we align in $\vec{z}$. Our goal is to determine the Chern number ($C$) in a two-torus normal to $\vec{z}$. For a 2D crystal, this two-torus ($T^2$) would be its Brillouin zone (BZ), while for a 3D crystal, the two-torus would be a submanifold of the BZ at fixed $k_z$. We find for a crystal with $\bar{n}$-fold rotational symmetry that the Chern number is determined modulo $\bar{n}$, by the rotational eigenvalues at various high-symmetry momenta. To define these rotational eigenvalues, it will be useful to recall certain notations from App. 1.3: we denote the
representation of $C_{n,\delta}$ (for any $n$ that divides $\bar{n}$) in the Bloch-wave orbital basis:

$$\hat{C}_{n,\delta}(k) = e^{-iD_n\delta \cdot k} U_{C_n,\delta},$$  

(4.11)

as well as in the occupied-band basis:

$$[\hat{\mathcal{C}}_{n,\delta}(D_n k + G, k)]_{ij} = \langle u_i, D_n k + G \vert V(-G) \hat{C}_{n,\delta}(k) \vert u_j, k \rangle.$$  

(4.12)

Here, $D_n$ represents an $n$-fold rotation in $\mathbb{R}^3$. A $C_n$-invariant momentum is defined by $\bar{k} = D_n k$ up to some reciprocal vector $(G(\bar{k}; D_n))$ that depends on $\bar{k}$ and $D_n$; the various $\bar{k}$ are illustrated in Fig. 4.10. The rotational eigenvalues $\{\lambda_{n,\delta,i}(\bar{k}) \vert i = 1, \ldots, n_{occ}\}$ are then defined as the eigenvalues of the matrix $\hat{\mathcal{C}}_{n,\delta}(\bar{k}, \bar{k})$. Now we are ready to state our results, with reference to Fig. 4.10: for space groups with

(i) $C_{6,\delta}$ symmetry,  

$$e^{-i\pi\mathcal{C}/3} = e^{i n_{occ}(0\delta \cdot k + F_\pi)} \prod_{i=1}^{n_{occ}} \lambda_{6,\delta,i}(\Gamma) \lambda_{3,2\delta,i}(K) \lambda_{2,3\delta,i}(M),$$  

(ii) $C_{4,\delta}$ symmetry,  

$$e^{-i\pi\mathcal{C}/2} = e^{i n_{occ}(4\delta \cdot k + F_\pi)} \prod_{i=1}^{n_{occ}} \lambda_{4,\delta,i}(\Gamma) \lambda_{2,2\delta,i}(X) \lambda_{4,\delta,i}(M),$$  

(iii) $C_{3,\delta}$ symmetry,  

$$e^{-i2\pi\mathcal{C}/3} = e^{i n_{occ}(3\delta \cdot k + F_\pi)} \prod_{i=1}^{n_{occ}} \lambda_{3,\delta,i}(\Gamma) \lambda_{3,\delta,i}(K_1) \lambda_{3,\delta,i}(K_2),$$  

(iv) $C_{2,\delta}$ symmetry,  

$$e^{-i\pi\mathcal{C}} = e^{i4 n_{occ}\delta \cdot k} \prod_{i=1}^{n_{occ}} \lambda_{2,\delta,i}(\Gamma) \lambda_{2,\delta,i}(X) \lambda_{2,\delta,i}(M) \lambda_{2,\delta,i}(Y).$$  

(4.13)

Here, $F = 0 \ (1)$ applies to integer-spin (resp. half-integer-spin) representations of the space group.

Figure 4.10: Rotationally-symmetric primitive cells with high-symmetry momenta indicated. Each cell in (a-d) has $C_{n,\delta}$ symmetry, with $\bar{n} = 6, 4, 3$ and 2 respectively. For each cell, a symmetrically-chosen Wilson loop is highlighted in blue, such that it encloses $1/\bar{n}$ of the cell.
It is worth commenting that our rotational-inversion formulae in Eq. (4.13) produces the absolute Chern number (mod $\bar{n}$) from knowledge of all occupied bands. It is often easier to compute a change in Chern number (mod $\bar{n}$) from knowledge of the inverting bands near the Fermi level, as we illustrate for our material class in Sec. 4.2.2.

Before we delve into the derivations, it pays to particularize the identity (1.29) for a reciprocal vector ($G$) that is orthogonal to $\vec{z}$:

$$\hat{C}_{n,\delta}(k) V(G) = V(D_n G) \hat{C}_{n,\delta}(k);$$

(4.14)
in particular, this identity holds for any of $\{G(\bar{k}; D_n)\}$. Lastly, we define a Wilson line on this two-torus as

$$[W_{k_2\leftarrow k_1}]_{mn} = \langle u_{m, k_2} \prod_k P(k) | u_{n, k_1} \rangle,$$

(4.15)
and from Eq. (1.26) deduce that

$$\hat{C}_{n,\delta}(D_n k_2, k_2) W_{k_2\leftarrow k_1} \hat{C}_{n,\delta}^{-1}(k_1, D_n k_1) = W_{D_n k_2\leftarrow D_n k_1}.$$

(4.16)

**QAHE criterion for systems with six-fold rotational symmetry**

The six-fold symmetry constrains the Berry curvature as $\mathcal{F}(k) = \mathcal{F}(D_6 k)$, and therefore the Berry flux enclosed by the Wilson loop of Fig. 4.10(a) is 1/6 of the total flux, i.e., $2\pi \hat{C}$. Then by Stoke’s theorem,

$$e^{-i\pi\hat{C}/3} = \det\left[ W_{\Gamma\leftarrow M_2} W_{M_2\leftarrow K} W_{K\leftarrow M_1} W_{M_1\leftarrow \Gamma} \right].$$

(4.17)

Into this equation, we insert two identities:

$$\hat{C}_{6,\delta}(\Gamma, \Gamma) W_{\Gamma\leftarrow M_1} \hat{C}_{6,\delta}^{-1}(M_1, M_2) = W_{\Gamma\leftarrow M_2},$$

(4.18)
and

$$\hat{C}_{3,2}\delta^{-1}(M_2, M_1) W_{M_1\leftarrow K} \hat{C}_{3,2}\delta(K, K) = W_{M_2\leftarrow K},$$

(4.19)
to obtain

\[ e^{-\pi C/3} = \det \begin{bmatrix} \hat{C}_{0,\delta}(\Gamma, \Gamma) \hat{C}_{2,3\delta}^{-1}(M_1, M_1) \hat{C}_{3,2\delta}(K, K) \end{bmatrix}. \] (4.20)

Applying that \( C_{2,3\delta}^2 \) is a \( 2\pi \) rotation combined with a \( 6\delta \) translation (if \( \delta \neq 0 \)),

\[ \hat{C}_{2,3\delta}^{-1}(M_1, M_1) = (-1)^F e^{i6k \cdot \delta} \hat{C}_{2,3\delta}(M_1, M_1), \] (4.21)

with \( F = 0(1) \) for integer-spin (half-integer spin) representations, and therefore

\[ e^{-\pi C/3} = e^{i\text{occ}(6k \cdot \delta + F\pi)} \det \begin{bmatrix} \hat{C}_{0,\delta}(\Gamma, \Gamma) \hat{C}_{2,3\delta}(M_1, M_1) \hat{C}_{3,2\delta}(K, K) \end{bmatrix}, \] (4.22)

which immediately leads to the first equation of (4.13).

**QAHE criterion for systems with four-fold rotational symmetry**

The other proofs are similar in structure, so we shall be terse. The four-fold symmetry constrains the Berry curvature as \( \mathcal{F}(k) = \mathcal{F}(D_4 k) \), and therefore

\[ e^{-i\pi C/2} = \det \begin{bmatrix} \mathcal{W}_{\Gamma \leftarrow Y} \mathcal{W}_{Y \leftarrow M} \mathcal{W}_{M \leftarrow X} \mathcal{W}_{X \leftarrow \Gamma} \end{bmatrix}, \] (4.23)

with the Wilson loop drawn in Fig. 4.10(b). Into this equation, we insert two identities:

\[ \hat{C}_{4,\delta}(\Gamma, \Gamma) \mathcal{W}_{\Gamma \leftarrow X} \hat{C}_{4,\delta}^{-1}(X, Y) = \mathcal{W}_{\Gamma \leftarrow Y} \] (4.24)

and

\[ \hat{C}_{4,\delta}^{-1}(Y, X) \mathcal{W}_{X \leftarrow M} \hat{C}_{4,\delta}(M, M) = \mathcal{W}_{Y \leftarrow M}, \] (4.25)

to obtain

\[ e^{-i\pi C/2} = \det \begin{bmatrix} \hat{C}_{4,\delta}(\Gamma, \Gamma) \hat{C}_{2,3\delta}^{-1}(X, X) \hat{C}_{4,\delta}(M, M) \end{bmatrix} \] (4.26)

Applying that \( C_{2,2\delta}^2 \) is a \( 2\pi \) rotation combined with a \( 4\delta \) translation (if \( \delta \neq 0 \)),

\[ \hat{C}_{2,3\delta}^{-1}(X, X) = (-1)^F e^{i4k \cdot \delta} \hat{C}_{2,3\delta}(X, X), \] (4.27)

and we arrive at the second equation of (4.13).
QAHE criterion for systems with three-fold rotational symmetry

The three-fold symmetry gives us that

\[ e^{-i2\pi C/3} = \det [ W_{\Gamma \to K_3} W_{K_3 \to K_2} W_{K_2 \to K_1} W_{K_1 \to \Gamma} ], \tag{4.28} \]

with the Wilson loop drawn in Fig. 4.10(c). Into this equation, we insert two identities:

\[ \check{C}_{3,\delta}(\Gamma, \Gamma) W_{\Gamma \to K_1} \check{C}_{3,\delta}^{-1}(K_1, K_3) = W_{\Gamma \to K_3} \tag{4.29} \]

and

\[ \check{C}_{3,\delta}^{-1}(K_3, K_1) W_{K_1 \to K_2} \check{C}_{3,\delta}(K_2, K_2) = W_{K_3 \to K_2}, \tag{4.30} \]

to obtain

\[ e^{-i2\pi C/3} = \det \left[ \check{C}_{3,\delta}(\Gamma, \Gamma) \check{C}_{3,\delta}^{-2}(K_1, K_1) \check{C}_{3,\delta}(K_2, K_2) \right] \tag{4.31} \]

Applying that \( C_{3,\delta}^3 \) is a \( 2\pi \) rotation combined with a \( 3\delta \) translation (if \( \delta \neq 0 \)),

\[ \check{C}_{3,\delta}^{-2}(K_1, K_1) = (-1)^F e^{i3\delta} \check{C}_{3,\delta}(K_1, K_1), \tag{4.32} \]

and we arrive at the third equation of (4.13).

QAHE criterion for systems with two-fold rotational symmetry

The two-fold symmetry gives us that

\[ e^{-i\pi C} = \det [ W_{\Gamma \to Y_2} W_{Y_2 \to M_2} W_{M_2 \to X} W_{X \to M_1} W_{M_1 \to Y_1} W_{Y_1 \to \Gamma} ], \tag{4.33} \]

with the Wilson loop drawn in Fig. 4.10(d). Into this equation, we insert the identities:

\[ \check{C}_{2,\delta}(\Gamma, \Gamma) W_{\Gamma \to Y_1} \check{C}_{2,\delta}^{-1}(Y_1, Y_2) = W_{\Gamma \to Y_2} \tag{4.34} \]

and

\[ \check{C}_{2,\delta}(M_2, M_1) W_{M_1 \to X} \check{C}_{2,\delta}^{-1}(X, X) = W_{M_2 \to X}, \tag{4.35} \]
to obtain

\[ e^{-i\pi \mathcal{C}} = \det[ \tilde{\mathcal{C}}_{2,\mathbf{C}}(\Gamma, \Gamma) \mathcal{C}_{2,\mathbf{C}}^{-1}(Y_1, Y_2) \mathcal{W}_{M_2 = M_1} \mathcal{C}_{2,\mathbf{C}}^{-1}(X, X) \mathcal{W}_{M_1 = Y_1} ]. \] (4.36)

It is worth noting that these matrix representations (e.g., \( \mathbf{C}_{2,\mathbf{C}} \), \( \mathbf{W}_{k' \leftarrow k} \)) depend on a particular decomposition of the occupied subspace into \( \{ u_{j,k} | j = 1, \ldots, n_{\text{occ}} \} \), but the final result is independent of this basis choice. Computation of Eq. (4.36) is eased if we now choose

\[ |u_{m,M_1}\rangle = V(2\pi \mathbf{y}) |u_{m,M_2}\rangle \text{ and } |u_{m,Y_1}\rangle = V(2\pi \mathbf{y}) |u_{m,Y_2}\rangle, \]

such that

\[ \mathcal{W}_{M_1 = Y_1} = \mathcal{W}_{M_2 = Y_2}, \quad \mathcal{C}_{2,\mathbf{C}}^{-1}(Y_1, Y_2) = \mathcal{C}_{2,\mathbf{C}}^{-1}(Y_2, Y_2) \quad \text{and} \quad \mathcal{C}_{2,\mathbf{C}}(M_2, M_1) = \mathcal{C}_{2,\mathbf{C}}(M_1, M_1). \] (4.37)

Further applying that \( \mathbf{C}_{2,\delta}^2 \) is a \( 2\pi \) rotation combined with a \( 2\delta \) translation (if \( \delta \neq 0 \)),

\[ \mathcal{C}_{2,\delta}^{-1}(k, \bar{k}) = (-1)^F e^{i2k \cdot \delta} \mathcal{C}_{2,\delta}(\bar{k}, \bar{k}), \] (4.38)

and we finally arrive at the last equation of (4.13).

### 4.2.2 Nontrivial mirror Chern number due to rotational inversion

Even where there is no net QAHE in the full occupied space, it is still possible to have a QAHE in one mirror subspace. [34] Here, we focus on glideless reflections, since the mirror Chern number is ill-defined for glide reflections. Our strategy is to identify space groups which allow simultaneous eigenstates of rotations and glideless reflections – only for these space groups may we apply our rotational-inversion formulae (Eq. (4.13)) to diagnose this mirror Chern number. It helps to distinguish between normal and screw rotations:

(i) Normal rotations and normal reflections only commute if the rotational and reflection axes coincide along \( \mathbf{z} \), by our convention; we denote such a reflection by \( M_z \). In any \( M_z \)-invariant plane, each eigenspace of \( M_z \) may be further block-diagonalized by \( C_{\alpha,\delta} \). Then the \( M_z \) Chern number may be determined modulo \( \bar{n} \) through Eq. (4.13), if we take the product of rotational eigenvalues only within one \( M_z \) subspace.
(ii) Screw rotations and normal reflections do not commute at all. However, if the reflection and rotational axes coincide, they commute modulo a translation, which in certain representations becomes a trivial phase factor. To elaborate, we have that $C_{n,\delta} M_z = t(2\delta) M_z C_{n,\delta}$ since $\delta$ lies along $\vec{z}$; this directionality is always true for screw rotations which, by definition, cannot be made screwless by a change in spatial origin. In a Bloch-wave representation, $t(2\delta) = \exp(-i2k \cdot \delta) = \exp(-i2k_z|\delta|)$. Since $\delta$ is not a lattice translation ($\bar{n}\delta$, however, must be), this phase factor is trivially identity only at $k_z = 0$. In this plane, we may then determine the mirror Chern number modulo $n$ through Eq. (4.13). A case in point is our material class KHgX, which is symmetric under a six-fold screw rotation $C_{6z,c\vec{z}/2}$, and also under the normal reflection $\bar{M}_z = M_{z,c\vec{z}/2}$. It is worth clarifying that this symmetry may either be represented as $\bar{M}_z$ (with the spatial origin at the inversion center of Fig. ??(a)), or as a pure reflection $M_z$ (with the origin displaced by $c\vec{z}/4$ from the inversion center); with either choice of origin, $M_z^2 = \bar{M}_z^2 = \bar{E}$ (a $2\pi$ rotation). Modulo six, the mirror Chern number ($C_e$) is determined by the rotational eigenvalues in the $M_z = +i$ subspace, which we list in Tab. 4.1. Given that the product of all eigenvalues in Tab. 4.1 is $\exp(-i2\pi/3)$, the first line of Eq. (4.13) informs us that $C_e = 2$ mod 6, which we confirm to be just 2 in the Wilson-loop calculation of Sec. 4.1.2.

While our method requires knowledge of all occupied bands, a shortcut to diagnosis is possible if one has a reference material that one knows to be trivial. For the sake of argument, let us assume we know KZnP to be trivial; its rotational eigenvalues are listed in Tab. 4.2 for direct confirmation. The difference between these two materials lies in a band inversion at $\Gamma$, where s-type $\Gamma_7$ and $\Gamma_9$ orbitals (found in KHgSb) interchange with p-type $\Gamma_{11}$ and $\Gamma_{12}$ (in KZnP). We would like to show that the rotational eigenvalues of these four bands alone determine the change in $C_e$ (mod 6) as a result of the band inversion. It is useful to define the discrete angular momentum ($J_z$) modulo six through $\lambda_{6z,c\vec{z}/2} \equiv \exp(-i\pi J_z/3)$; the tables inform us that $\Gamma_7$ transform as $J_z = -1/2$, $\Gamma_9$ as $+5/2$, $\Gamma_{11}$ as $+3/2$ and $\Gamma_{12}$ as $-3/2$ – the net change in angular momentum is $\Delta J_z = 2$. Given that Eq.
(4.13) applies individually to KZnP and KHgSb, we divide one equation by the other to obtain $\Delta C_e = \Delta J_z = 2 \mod 6$.

$$\Delta C_e = \Delta J_z = 2 \mod 6.$$  

\begin{table}[h]
\begin{tabular}{|c|c|c|c|}
\hline
No. & $\Gamma(C_6)$ & $K(C_3)$ & $M(C_2)$ \\
\hline
1 & $\Gamma_{10}(-i\omega^*)$ & $K_6(-1)$ & $M_3(+i)$ \\
2 & $\Gamma_{8}(+i\omega^*)$ & $K_5(-\omega)$ & $M_4(-i)$ \\
3 & $\Gamma_{9}(+i\omega)$ & $K_4(-\omega^*)$ & $M_3(+i)$ \\
4 & $\Gamma_{7}(-i\omega)$ & $K_4(-\omega^*)$ & $M_4(-i)$ \\
5 & $\Gamma_{10}(-i\omega^*)$ & $K_6(-1)$ & $M_4(-i)$ \\
6 & $\Gamma_{8}(+i\omega^*)$ & $K_4(-\omega^*)$ & $M_3(+i)$ \\
\hline
\end{tabular}
\caption{Rotational analysis of KHgSb. For the six occupied bands in the $M_z = +i$ subspace, we list their representation labels and their rotational eigenvalues (in brackets). Note $\omega = \exp(i2\pi/3)$, and the product of all eigenvalues in this table is $\omega^{-4}$.}
\end{table}

\begin{table}[h]
\begin{tabular}{|c|c|c|c|}
\hline
No. & $\Gamma(C_6)$ & $K(C_3)$ & $M(C_2)$ \\
\hline
1 & $\Gamma_{10}(-i\omega^*)$ & $K_6(-1)$ & $M_3(+i)$ \\
2 & $\Gamma_{8}(+i\omega^*)$ & $K_5(-\omega)$ & $M_4(-i)$ \\
3 & $\Gamma_{9}(+i\omega)$ & $K_4(-\omega^*)$ & $M_3(+i)$ \\
4 & $\Gamma_{8}(+i\omega^*)$ & $K_4(-\omega^*)$ & $M_4(-i)$ \\
5 & $\Gamma_{11}(-i)$ & $K_6(-1)$ & $M_4(-i)$ \\
6 & $\Gamma_{12}(+i)$ & $K_4(-\omega^*)$ & $M_3(+i)$ \\
\hline
\end{tabular}
\caption{Rotational analysis of KZnP. For the six occupied bands in the $M_z = +i$ subspace, we list their representation labels and their rotational eigenvalues (in brackets). Note $\omega = \exp(i2\pi/3)$, and the product of all eigenvalues in this table is 1.}
\end{table}

### 4.3 Discussion

**Discussion** Spatial symmetries have played a crucial role in the topological classification of insulators. [5, 7, 19, 36, 62, 63] To date, all experimentally-tested topological insulators have relied on symmorphic space groups. [7,35,39,55–57] In KHg$X$ ($X$=As, Sb and Bi) and related compounds RbHg$X$ and NaHgSb, we propose the first family of insulators with non-symmorphic topology, in the hope of stimulating interest in an experimentally barren field.

Our time-reversal-invariant theory of KHg$X$ complements previous theoretical proposals
with magnetic, non-symmorphic space groups. [36, 63–66] To describe KHgX, we introduced a quantized polarization which naturally describes glide-symmetric crystals; while the standard polarization relates to the Abelian Berry connection, [27,29,47] our proposed polarization depends instead on the non-Abelian Berry connection. [26,51,67] Additionally, KHgX uniquely exemplifies a ‘rotationally-inverted’ insulator; we have described a general strategy to search for such materials in all space groups. It is worth mentioning that KHgX represents one among many possible topologies within its space group, e.g., another non-trivial example is illustrated in Fig. 4.1(c). The full classification is more mathematical and will be presented in the next Chapter.
Chapter 5

Non-symmorphic Topology and Group Cohomology in Band Insulators

Motivated by the KHgX material class that we proposed last Chapter, we present a complete classification of spin-orbit-coupled insulators with a similar space group. These insulators are found to be ‘piecewise topological’, in the sense that sub-topologies describe the different high-symmetry submanifolds of the Brillouin zone, and the various sub-topologies must be pieced together to form a globally consistent topology. The sub-topologies that we discovered include: (i) a glide-analog of the quantum spin Hall effect \[3, 68\], as illustrated in Fig. 5.1(a); we further propose a realization with Dirac-semimetallic \[69\] Na$_3$Bi under pressure, (ii) an hourglass-zigzag topology (exemplified by KHgX and illustrated in Fig. 5.1(b)), and (iii) quantized non-Abelian polarizations. To construct piecewise topologies, we propose a general methodology through Wilson loops, \[50, 51\] which represent parallel transport in quasimomentum space. \[29\] Our classification method is shown to be efficient and geometrically intuitive – piecing together sub-topologies reduces to a problem of matching curves. Our final result is summarized in Tab. 5.1.
Figure 5.1: Examples of possible piecewise topologies, as illustrated by the surface band-structures along a bent high-symmetry line. (a) describes a ‘glide spin Hall effect’ (along $\tilde{Z}\tilde{\Gamma}$), and an odd mirror Chern number (along $\tilde{\Gamma}\tilde{X}$); these two sub-topologies must be pieced together at their intersection point $\tilde{\Gamma}$. (b) describes an hourglass-zigzag topology ($\tilde{X}\tilde{U}\tilde{Z}\tilde{\Gamma}$), and an even mirror Chern number ($\tilde{\Gamma}\tilde{X}$). (c) A trivial topology is shown for comparison.

Table 5.1: Classification of piecewise topological insulators with time-reversal, spatial-inversion and Pma2 symmetries. A glide-projected polarization ($\mathcal{P}_\eta^g$) distinguishes between two families of insulators: $\mathcal{P}_\eta^g=0$ ($=\frac{e}{2}$) is characterized the absence (resp. presence) of the ‘glide spin Hall effect’. The $\mathcal{P}_\eta^g=0$ family is further sub-classified by two non-Abelian polarizations: $Q_0 \in \mathbb{Z}_2$ and $Q_\pi \in \mathbb{Z}_2$, and a mirror Chern number ($C_e$) that is constrained to be even; where $Q_0 \neq Q_\pi$, the insulator manifests an hourglass-zigzag topology. The $\mathcal{P}_\eta^g=e/2$ family is sub-classified by $Q_\pi \in \mathbb{Z}_2$ and odd $C_e$.

<table>
<thead>
<tr>
<th>$\mathcal{P}_\eta^g$</th>
<th>$Q_0$</th>
<th>$Q_\pi$</th>
<th>$C_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$=0$</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
<td>$2\mathbb{Z}$</td>
</tr>
<tr>
<td>$=e/2$</td>
<td>$-$</td>
<td>$\mathbb{Z}_2$</td>
<td>$2\mathbb{Z}+1$</td>
</tr>
</tbody>
</table>

The non-symmorphic topologies that we introduce are naturally described by group cohomology. This language arises when we generalize the traditional notion of symmetry as a space-time transformation – we instead encounter ‘symmetry’ operators that combine both space-time transformations and quasimomentum translations. These ‘symmetries’ generate an extension of the ordinary crystal group ($G_s$) by Wilson loops, i.e., the Wilson loop becomes an element in a projective representation of $G_s$. Our finding generalizes the construction of non-symmorphic space groups, which extend point groups by real-space translations. [6] Here, we further extend non-symmorphic groups by reciprocal translations, thus placing real and quasimomentum space on equal footing. The different extensions are classified by the second cohomology group, and correspond to different band sub-topologies.

A consequence of this projective representation is an atypical bulk-boundary corre-
spondence for symmetry-protected topological insulators. This correspondence describes a one-to-one mapping between topological numbers that describe bulk wavefunctions and surface topological numbers [52] – such a mapping exists if the bulk and surface share an ‘edge symmetry’ which protects the topology. In our case study, the edge symmetry is projectively represented in the bulk, where quasimomentum provides the parameter space for parallel transport; on a surface with reduced translational symmetry, the same symmetry is represented ordinarily. In contrast, all known symmetry-protected correspondences [50] rely on the identity between bulk and surface representations; our work explains how a correspondence arises even where such identity is absent.

The outline of this Chapter: In Sec. 5.1, we review the Wilson loop and the bulk-boundary correspondence of topological insulators; the notion of a partial correspondence is introduced, and exemplified with our non-symmorphic study. The method of Wilson loops is then used to construct and classify a piecewise topological insulator in Sec. 5.2; here, we introduce the glide spin Hall effect and propose a material realization in pressured Na$_3$Bi. Our topological classification relies on extending the symmetry group by Wilson loops, as we elaborate in Sec. 5.3; the application of group cohomology in band theory is introduced here. The rest of the Chapter contains some technical derivations, as well as an introduction to group cohomology.

(5.4) We derive how symmetries of the Wilson loop are represented, and their implications for the ‘rules of the curves’, as summarized in Tab. 5.2 and 5.3. The first few Sections deal with ordinary symmetry representations along $\tilde{X}\tilde{\Gamma}\tilde{Z}\tilde{U}$, while the last derives the projective representations along $\tilde{X}\tilde{U}$.

(5.5) We prove the four-fold connectivity of Hamiltonian bands, in spin systems with minimally time-reversal and glide-reflection symmetries. This proof is used in the topological classification of Sec. 5.2.2.
(5.6) We introduce group extensions by Wilson loops, as well as rederive the extended algebra in Sec. 5.3 from a group-theoretic perspective.

We end with a few remarks in Sec. 5.7.

5.1 Wilson loops and the bulk-boundary correspondence

In Sec. 5.1.1, we introduce the loop geometry that is assumed throughout this Chapter. The connection of Wilson loops with the geometric theory of polarization is summarized in Sec. 5.1.2. There, we also introduce the notion of a partial bulk-boundary correspondence, which our non-symmorphic insulator exemplifies.

5.1.1 Review of Wilson loops

In this Chapter, we consider only a family of Wilson loops parametrized by \( k_q = (k_x \in [-\pi/\sqrt{3}a, +\pi/\sqrt{3}a], k_z \in [-\pi/c, +\pi/c]) \), where for each loop \( k_q \) is fixed while \( k_y \) is varied over a non-contractible circle (colored red in Fig. 4.7(a)). We then label each Wilson loop as \( \mathcal{W}(k_q) \) and denote its eigenvalues by \( \exp[i\theta_{n,k_q}] \) with \( n = 1, \ldots, n_{\text{occ}} \). Note that \( k_q \) also parametrizes the 010-surface bands, hence we refer to \( k_q \) as a surface wavevector; here and henceforth, we take the unconventional ordering \( k = (k_y, k_x, k_z) = (k_y, k_q) \). To simplify notation in the rest of the Chapter, we reparametrize the rectangular primitive cell of Fig. 4.7 to be a cube of dimension \( 2\pi \), i.e., \( k_x = \pi/\sqrt{3}a \rightarrow k_x = \pi, k_y = 2\pi/a \rightarrow k_y = \pi, \) and \( k_z = \pi/c \rightarrow k_z = \pi \). The time-reversal-invariant \( k_q \) are then labelled as: \( \tilde{\Gamma} = (0,0), \tilde{X} = (\pi,0), \tilde{Z} = (0,\pi) \) and \( \tilde{U} = (\pi,\pi) \). For example, \( \mathcal{W}(\tilde{\Gamma}) \) would correspond to a loop parametrized by \( (k_y,0,0) \).
5.1.2 Bulk-boundary correspondence of topological insulators

The bulk-boundary correspondence describes topological similarities between the Wilson loop and the surface bandstructure. To sharpen this analogy, we refer to the eigenvectors of \( W(k_q) \) as forming Wilson bands with energies \( \theta_{n,k_q} \). The correspondence may be understood in two steps:

(i) The first is a spectral equivalence between \( (-i/2\pi)\log W(k_q) \) and the projected position operator \( P_\perp(k_q)\hat{y}P_\perp(k_q) \), where

\[
P_\perp(k_q) = \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} P(k_y,k_q)
\]

projects to all bands with surface wavevector \( k_q \). For the position operator \( \hat{y} \), we have chosen natural units of the lattice where \( 1 \equiv a/2 \) is the translational period in \( \hat{y} \). Denoting the eigenvalues of \( P_\perp(k_q)\hat{y}P_\perp(k_q) \) as \( y_{n,k_q} \), the two spectra are related as \( y_{n,k_q} = \theta_{n,k_q}/2\pi \) modulo one. [51] Some intuition about the projected position operator may be gained from studying its eigenfunctions; they form a set of hybrid functions \( \{|k_q,n\rangle | n \in \{1,2,\ldots,n_{occ}\} \} \) which maximally localize in \( \hat{y} \) (as a Wannier function) but extend in \( \hat{x} \) and \( \hat{z} \) (as a Bloch wave with momentum \( k_q = (k_x,k_z) \)). In this Bloch-Wannier (BW) representation, [50] the eigenvalue \( (y_{n,k_q}) \) under \( P_\perp\hat{y}P_\perp \) is merely the center-of-mass coordinate of the BW function \( (|n,k_q\rangle) \). [51,70] Due to the discrete translational symmetry of \( P_\perp \), each of \( \{y_{n,k_q}\} \) represents a family of BW functions which are related by integer translations. The Abelian polarization \( (P/e) \) is defined as the net displacement of BW functions: [47–49]

\[
\frac{P_{k_q}}{e} = \text{Tr} \left[ P_\perp(k_q) \hat{y} P_\perp(k_q) \right] \mod 1
= \frac{1}{2\pi} \sum_{j=1}^{n_{occ}} \theta_{j,k_q} \mod 1.
\]

(ii) The next step is an interpolation [52,53] between \( P_\perp\hat{y}P_\perp \) and an open-boundary Hamiltonian \( (H_s) \) with a surface termination. Given a surface termination, we refer to the subset of bulk symmetries which are preserved by that surface as edge symmetries. Since an interpolation can be found which preserves the edge symmetries, we expect that both \( P_\perp\hat{y}P_\perp \)
(equivalently, \(\log W\)) and \(H_s\) share topological features that are protected by said symmetries. A simple example is the quantum spin Hall (QSH) insulator, where both the Berry-Zak phases and the boundary bandstructure exhibit a zigzag pattern that connects every Kramers subspace. [51,70,71] Here, it might be taken for granted that the representation \((T^2 = -I)\) of the edge symmetry is identical for both \(H_s\) and \(W\); the invariance of \(T^2 = -I\) throughout the interpolation accounts for the persistence of Kramers degeneracies, and consequently for the entire zigzag topology. The QSH phase thus exemplifies a total bulk-boundary correspondence, where the entire set of boundary topologies (i.e., topologies that are consistent with the edge symmetries of \(H_s\)) is in one-to-one correspondence with the entire set of \(W\)-topologies (i.e., topologies which are consistent with symmetries of \(W\), of which the edge symmetries form a subset). One is then justified in inferring the topological classification purely from the representation theory [36,62,72] of surface wavefunctions.

While this surface-centric approach is technically easier than the representation theory of Wilson loops, it ignores the bulk symmetries that are spoilt by the boundary. On the other hand, \(W\)-topologies encode said symmetries, and are therefore more reliable in a topological classification. In some cases, [51,67,73,74] these bulk symmetries enable \(W\)-topologies that have no boundary analog. Simply put, some topological phases do not have robust boundary states, a case in point being the \(Z\) topology of 2D inversion-symmetric insulators, which we describe in Chap. 6. In our non-symmorphic case study, it is an out-of-surface translational symmetry \((t_\perp)\) that disables a \(W\)-topology, and consequently a naive surface-centric approach would over-predict the topological classification – this exemplifies a partial bulk-boundary correspondence. As we will clarify, the \(t_\perp\) symmetry distinguishes between two representations of the same edge symmetries: an ordinary representation in \(H_s\), and a projective one in \(W\). To state the conclusion upfront, the projective representation rules out a glide spin Hall topology that would otherwise be allowed in the ordinary representation. This discussion motivates a careful determination of the \(W\)-topologies in Sec. 5.2.
5.2 Constructing a piecewise topological insulator by Wilson loops

We would like to classify time-reversal-invariant insulators with the non-symmorphic edge symmetry $Pma2$ and a bulk spatial-inversion symmetry; our discussion applies to but is not limited to the space group of the KHg$X$ material class. Recall from Chap. 4 that $Pma2$ is the symmetry of the 010 surface of KHg$X$, and the edge group is generated by two reflections: glideless $\bar{M}_z$ and glide $\bar{M}_x$. Our final classification in Tab. 5.1 relies on topological invariants that we briefly introduce here, deferring a detailed explanation to the sub-sections below. The invariants are: (i) the mirror Chern number ($C_e$) in the $k_z = 0$ plane, (ii) the quadruplet polarization $Q_0$ ($Q_\pi$) in the $k_x = 0$ glide plane (resp. $k_x = \pi$), and (iii) the glide polarization $P_\eta^\theta = 0$ ($e/2$) indicates the absence (resp. presence) of the glide spin Hall effect in the $k_x = 0$ plane.

Our strategy for classification is simple: we first derive the symmetry constraints on the Wilson-loop spectrum, then enumerate all topologically distinct spectra that are consistent with these constraints. Pictorially, this amounts to understanding the rules obeyed by curves (the Wilson bands), and connecting curves in all possible legal ways; we do these in Sec. 5.2.1 and 5.2.2 respectively. In Sec. 5.2.3, we propose that Na$_3$Bi realizes a glide spin Hall effect under pressure.

5.2.1 Local rules of the curves

We consider how the symmetries constrain the Wilson loop $W(k_n)$, with $k_n$ lying on the high-symmetry line $\Gamma \bar{X} \bar{U} \bar{Z} \Gamma$; note that $\bar{\Gamma} \bar{Z}$ and $\bar{X} \bar{U}$ are glide mirror lines, while $\bar{\Gamma} \bar{X}$ and $\bar{Z} \bar{U}$ are glide-less mirror lines. We are interested only in those symmetries which map $k_n \rightarrow k_n$ up to a surface reciprocal vector, e.g., we would be interested in $T \bar{X}$ and $T \bar{M}_z$ at any point along $\bar{\Gamma} \bar{X}$, but $T$ matters only at the time-reversal-invariant $k_n$. Along $\bar{\Gamma} \bar{X}$, we
omit discussion of other symmetries (e.g., $TC_{2y}$) which also map $k_n \rightarrow k_n$, because they do not provide additional constraints. For each symmetry, only three of its characteristics influence the connectivity of curves:

(i) Does the symmetry map the Wilson energy as $\theta \rightarrow \theta$ or $\theta \rightarrow -\theta$?
(ii) Does the symmetry result in Kramers-like degeneracy?
(iii) How does the symmetry transform the mirror eigenvalues of the Wilson bands?

(i) and (ii) are determined by how the symmetry constrains the Wilson loop. We say that a symmetry represented by $T_{\pm}$ is time-reversal-like if

$$T_{\pm} W(k_n) T_{\pm}^{-1} = W(k_n)^{-1},$$

with $T_{\pm} i T_{\pm}^{-1} = -i$, and $T_{\pm}^2 = \pm I.$

(5.3)

Both $T_{\pm}$ map the Wilson energy as $\theta \rightarrow \theta$, but only $T_-$ symmetries guarantee a Kramers-like degeneracy. Similarly, a symmetry represented by $U$ is particle-hole-like if

$$U W(k_n) U^{-1} = W(k_n), \quad \text{with} \quad U i U^{-1} = -i,$$

(5.4)

i.e., $U$ maps the Wilson energy as $\theta \rightarrow -\theta$. (iii) is determined by the commutation relation between the symmetry in question and the relevant reflection. We have derived (i-iii) in App. 5.4, and here we just summarize our results in Tab. 5.2 and 5.3. For example, the top left entry of the first table describes the effect of $TI$ along the $\tilde{\Gamma} \tilde{X}$. The notation $U : \lambda_x \rightarrow -\lambda_x$ means that (a) $TI$ imposes a particle-hole symmetric spectrum, and (b) two states related by $TI$ have opposite eigenvalues under $\tilde{M}_x$. Note these eigenvalues fall into either of two momentum-dependent branches, as follows from $\tilde{M}_x^2 = t(\vec{z}) \tilde{E}$, with $\tilde{E}$ denoting a $2\pi$ rotation and $t$ a lattice translation. Explicitly, the Bloch representation of $\tilde{M}_x$ squares to $-\exp(-ik_z)$, which implies for the glide eigenvalues: $\lambda_x(k_z) = \pm i\exp(-ik_z/2)$. On the other hand, $\tilde{M}_z^2 = \tilde{E}$ implies two momentum-independent branches for the eigenvalues of $\tilde{M}_z$: $\lambda_z = \pm i$. 
Table 5.2: Symmetry constraints of the Wilson bands at generic points along the mirror lines. $\mathcal{T}_\pm (\mathcal{U})$ refers to a time-reversal-like (resp. particle-hole-like) symmetry, as defined in Eq. (5.3) and (5.4). For $j \in \{x,z\}$, $\lambda_j$ is the eigenvalue of the reflection $\tilde{M}_j$, which falls into one of two branches: $\lambda_z = \pm i$, and $\lambda_x(\alpha) = \pm i \exp(-i\alpha/2)$. Along $k_x = 0$, $\lambda_x$ is momentum-dependent; along $k_x = \pi$, it is energy-dependent as well, that is, $\lambda_x(k_x + \theta)$ is the glide eigenvalue of a Wilson band at momentum $k_z$ and energy $\theta$.

<table>
<thead>
<tr>
<th></th>
<th>$k_x = 0 (\tilde{\Gamma} \tilde{Z})$</th>
<th>$k_x = \pi (\tilde{X} \tilde{U})$</th>
<th>$k_z = 0 (\tilde{\Gamma} \tilde{X})$</th>
<th>$k_z = \pi (\tilde{Z} \tilde{U})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T \tilde{I}$</td>
<td>$\mathcal{U} : \lambda_z(k_z) \rightarrow -\lambda_z(k_z)$</td>
<td>$\mathcal{U} : \lambda_x(k_x + \theta) \rightarrow -\lambda_x(k_x - \theta)$</td>
<td>$\mathcal{U} : \lambda_z \rightarrow -\lambda_z$</td>
<td>$\mathcal{U} : \lambda_z \rightarrow +\lambda_z$</td>
</tr>
<tr>
<td>$T \tilde{M}_z$</td>
<td>$\mathcal{T}_+ : \lambda_x(k_z) \rightarrow +\lambda_x(k_z)$</td>
<td>$\mathcal{T}_- : \lambda_x(k_x + \theta) \rightarrow +\lambda_x(k_x + \theta)$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$T \tilde{M}_x$</td>
<td>-</td>
<td>-</td>
<td>$\mathcal{T}_+ : \lambda_z \rightarrow +\lambda_z$</td>
<td>$\mathcal{T}_- : \lambda_z \rightarrow -\lambda_z$</td>
</tr>
</tbody>
</table>

Table 5.3: Time-reversal constraint of the Wilson bands at surface wavevectors satisfying $\mathbf{k}_i = (k_x, k_z) = -\mathbf{k}_i$ modulo a reciprocal vector.

<table>
<thead>
<tr>
<th></th>
<th>$\tilde{\Gamma} = (0,0)$</th>
<th>$\tilde{X} = (\pi,0)$</th>
<th>$\tilde{Z} = (0,\pi)$</th>
<th>$\tilde{U} = (\pi,\pi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>$\mathcal{T}_- : \lambda_z \rightarrow -\lambda_z, \lambda_x(k_z) \rightarrow -\lambda_x(k_z)$</td>
<td>$\mathcal{T}_- : \lambda_z \rightarrow -\lambda_z, \lambda_x(k_x + \theta) \rightarrow -\lambda_x(k_x + \theta)$</td>
<td>$\mathcal{T}_- : \lambda_z \rightarrow -\lambda_z, \lambda_x(k_z) \rightarrow +\lambda_x(k_z)$</td>
<td>$\mathcal{T}_- : \lambda_z \rightarrow -\lambda_z, \lambda_x(k_x + \theta) \rightarrow +\lambda_x(k_x + \theta)$</td>
</tr>
</tbody>
</table>
Since the spectra of \((-i/2\pi)\log W(k)\) and \(P_{\perp}(k)\hat{y}P_{\perp}(k)\) coincide, we may alternatively derive these tables in the polarization perspective. For illustration, consider how \(T\mathcal{I}\) inverts all spatial coordinates but transforms any momentum to itself – the particle-hole symmetry of \(W(k)\) is thus interpreted as a spatial-inversion symmetry of \(P_{\perp}(k)\hat{y}P_{\perp}(k)\): \(y_{n,k} \rightarrow -y_{n,k}\). Moreover, all eigenstates of \(P_{\perp}(0,k_z)\hat{y}P_{\perp}(0,k_z)\) may simultaneously be labelled by \(\bar{M}_x\). That \(T\mathcal{I}\) maps \(\lambda_x \rightarrow -\lambda_x\) then follows from \(\bar{M}_xT\mathcal{I} = t(\hat{z})T\mathcal{I}\bar{M}_x\). In analogous fashion, we may derive the other tabulated constraints except along \(\tilde{X}\tilde{U}\). This exception arises because \(\bar{M}_x\) is not a symmetry of any bulk wavevector that projects to \(\tilde{X}\tilde{U}\), despite being a symmetry of any surface wavevector along \(\tilde{X}\tilde{U}\). Instead, \(\bar{M}_x\) relates two bulk momenta which are separated by half a reciprocal vector, i.e., \(\bar{M}_x : (k_y,\pi,k_z) \rightarrow (k_y,-\pi,k_z) = (k_y + \pi,\pi,k_z) - \hat{b}_2\), as illustrated in Fig. 4.7(b). It follows that \(P_{\perp}(\pi,k_z)\) is not invariant under \(\bar{M}_x\), and therefore the eigenstates of \(P_{\perp}(\pi,k_z)\hat{y}P_{\perp}(\pi,k_z)\) do not have a symmetry quantum number. However, a generalized notion of a quantum number remains, provided we let the ‘symmetry’ eigenvalue depend on energy as well:

\[
\lambda_x(\theta + k_z) = \eta i \exp \left[-i(\theta + k_z)/2\right] \text{ with } \eta = \pm 1.
\]

In the Wilsonian language, \(\lambda_x(\theta + k_z)\) is the ‘symmetry’ eigenvalue of a Wilson band at surface momentum \((\pi,k_z)\) and energy \(\theta\). The corresponding ‘symmetry’ operation actually combines a spatial transformation with parallel transport, as we elaborate in Sec. 5.3. The reader who is most interested in the topological classification may continue to Sec. 5.2.2, where we begin matching curves to determine possible topologies.

### 5.2.2 Connecting curves in all possible legal ways

Our goal here is to determine the possible topologies of curves (Wilson bands), which are piecewise smooth on the high-symmetry line \(\bar{\Gamma}\bar{X}\bar{U}\bar{Z}\bar{\Gamma}\). We first analyze each momentum interval separately, by evaluating the available sub-topologies within each of \(\bar{\Gamma}\bar{Z}, \bar{Z}\bar{U},\) etc. The various sub-topologies are then combined to a full topology, by a program of matching curves at the intersection points (e.g., \(\bar{Z}\)) between momentum intervals.
Since our program here is to interpolate and match curves (Wilson bands), it is important to establish just how many Wilson bands must be connected. A combination of symmetry, band continuity and topology dictates this answer to be a multiple of four. Since the number \( n_{\text{occ}} \) of occupied Hamiltonian bands is also the dimension of the Wilson loop, it suffices to show that \( n_{\text{occ}} \) is a multiple of four. Indeed, this follows from our assumption of insulation, and a property of connectedness between sets of Hamiltonian bands. For spin systems with \textit{minimally} time-reversal and glide-reflection symmetries, we prove in App. 5.5 that Hamiltonian bands divide into sets of four which are individually connected, i.e., in each set there are enough contact points to travel continuously through all four branches. The lack of gapless excitations in an insulator then implies that a connected quadruplet is either completely occupied, or unoccupied.

**Interpolating curves along the glide line \( \tilde{\Gamma} \tilde{Z} \)**

The rules as obtained from our tables are:

(a) There are two flavors of curves (illustrated as blue solid and blue dashed), corresponding to two branches of the glide eigenvalue. Only crossings between solid and dashed curves are robust, in the sense of being movable but unremovable.

(b) At any point along \( \tilde{\Gamma} \tilde{Z} \), there is a particle-hole symmetry with conjugate bands belonging in opposite glide branches. Pictorially, \([\theta, \text{blue solid}] \leftrightarrow [-\theta, \text{blue dashed}]\).

(c) At \( \tilde{\Gamma} \), each solid curve is degenerate with a dashed curve, while at \( \tilde{Z} \) the degeneracies are solid-solid and dashed-dashed. These constraints are boundary conditions in our curve-interpolation problem.

Given these rules, there are three distinct connectivities, which we describe in turn: (i) a zigzag connectivity defines the glide spin Hall effect (GSHE), and (ii) two configurations of
hourglasses are distinguished by a quadruplet polarization ($Q_0$).

(i) As illustrated in Fig. 5.2(a–e), the GSHE describes a zigzag connectivity over $\tilde{\Gamma} \tilde{Z}$, where each cusp of the zigzag corresponds to a Kramers-degenerate subspace. While Fig. 5.2(c–d) is not obviously zigzag, they are smoothly deformable to Fig. 5.2(a) which clearly is. A unifying property of all five figures (a–e) is spectral flow: the GSHE is characterized by Wilson bands which robustly interpolate across the maximal energy range of $2\pi$. Despite describing the band topology over all of $\tilde{\Gamma} \tilde{Z}$, the GSHE is solely determined by a polarization invariant ($\mathcal{P}_\eta^\tilde{\Gamma}$) at a single point ($\tilde{\Gamma}$).

**Definition of $\mathcal{P}_\eta^\tilde{\Gamma}$**: Consider the $k_x=k_z=0$ circle of the 3D Brillouin zone. Each point here has the glide symmetry $\tilde{M}_x$, and the Bloch waves divide into two glide subspaces labelled by $\eta=\pm$, according to their eigenvalue under $\tilde{M}_x$: $\lambda_x = \eta i$. This allows us to define an Abelian polarization ($\mathcal{P}_\eta^\tilde{\Gamma}/e$) as the net displacement of Bloch-Wannier functions in either $\eta$ subspace:

\[
\mathcal{P}_\eta^\tilde{\Gamma}/e = \text{Tr} \left[ P_\eta^\tilde{\Gamma}(\tilde{\Gamma}) \hat{y} P_\eta^\tilde{\Gamma}(\tilde{\Gamma}) \right] \mod 1
\]

\[
= \frac{1}{2\pi} \sum_{j=1}^{n_{occ}/2} \theta^\eta_{j,\tilde{\Gamma}/e} \mod 1.
\]  

(5.6)
Here, the superscript $\eta$ indicates a restriction to the $\vec{M}_x = \eta$, occupied subspace; $\{\exp(i\theta^\eta)\}$ are the eigenvalues of the Wilson loop $W^\eta(\vec{\Gamma})$, and the second equality follows from the spectral equivalence introduced in Sec. 5.1. We have previously determined in this Section that $n_{\mathrm{occ}}$ is a multiple of four, and therefore there is always an even number ($n_{\mathrm{occ}}/2$) of Wilson bands in either $\eta$ subspace. Furthermore, $P^\eta_+ = P^\eta_-$ modulo $e$ follows from time reversal relating $\theta^\eta_+ = \theta^\eta$; cf. Tab. 5.3.

We claim that the effect of spatial inversion ($I$) symmetry is to quantize $P^\eta_+$ to 0 and $e/2$, which respectively corresponds to the absence and presence of the GSHE. To demonstrate this, (i-a) we first relate the boundary conditions at $\vec{\Gamma}$ to the invariant $P^\eta_+$, then (i-b) determine the possible boundary conditions at $\vec{Z}$. (i-c) These boundary conditions determine two classes of interpolating curves along $\vec{\Gamma}\vec{Z}$, which are distinguished by spectral flow.

(i-a) To prove the quantization of $P^\eta_+$, consider how each glide subspace is individually invariant under $I$. This invariance follows from

$$\vec{M}_x I = t(\vec{z}) I \vec{M}_x,$$

leading to the representative commutivity of $I$ and $\vec{M}_x$ where $k_z = 0$. From Tab. 5.2 and 5.3, we further obtain that $I$ maps $\theta^\eta_+ \rightarrow -\theta^\eta_+ \mod 2\pi$. $\theta^\eta_+$ and $-\theta^\eta_+$ may correspond either to two distinct Wilson bands (an inversion doublet), or to the same Wilson band (an inversion singlet at $\theta^\eta_+ = 0$ or $\pi$). Since there are an even number of Wilson bands in each $\eta$ subspace, a 0-singlet is always accompanied by a $\pi$-singlet — such a singlet pair produces the only non-integral contribution to $P^\eta_+ (= e/2)$; the absence of singlets corresponds to $P^\eta_+ = 0$. These two cases correspond to two classes of boundary conditions at $\vec{\Gamma}$.

(i-b) What is left to determine the possible boundary conditions at $\vec{Z}$. We find here only one class of boundary conditions, i.e., any one boundary condition may be smoothly deformed into another, indicating the absence of a nontrivial topological invariant at $\vec{Z}$. Indeed, the same non-symmorphic algebra (Eq. (5.7)) has different implications where $k_z = \pi$: now $I$
relates Wilson bands in opposite glide subspaces, i.e., \( I : \theta^n_0 \rightarrow \theta^{-n}_0 = -\theta^n_0 \). Consequently, the total polarization \( \mathcal{P}_2 \) vanishes modulo \( e \), and the analogous \( \mathcal{P}_2^n \) is well-defined but not quantized. With the additional constraint by \( T \) (see Tab. 5.3), any Kramers pair belongs to the same glide subspace, while particle-hole-related pairs belong to different glide subspaces.

(i-c) Having determined all boundary conditions, we proceed to the interpolation. For simplicity, this is first performed for the minimal number (four) of Wilson bands; the two energy functions in each \( \eta \) subspace are defined as \( \theta^n_{\eta, k} \) and \( \theta^n_{\eta, k'} \). If \( \mathcal{P}_\Gamma^n = e/2 \), the boundary conditions are

\[
\theta^n_{\eta, \Gamma} = 0, \quad \theta^n_{\eta, \Gamma} = \pm \pi, \quad \text{and} \quad \theta^{n, -n}_{\eta, \Gamma} = \theta^{n, -n}_{\eta, \Gamma} = \theta^{n, -n}_{\eta, \Gamma} = \theta^{n, -n}_{\eta, \Gamma}.
\]

In one of the glide subspaces (say, \( \bar{\eta} \)), the two energy functions sweep out an energy interval that contains at least \([0, \pi]\) (e.g., Fig. 5.2(a)), but may contain more (e.g., Fig. 5.2(c)). The particle-hole symmetry (due to \( T \bar{T} \)) further imposes that the other two energy functions (in \(-\bar{\eta}\)) sweep out at least \([-\pi, 0]\) – the net result is that the entire energy range is swept; this spectral flow is identified with the GSHE. If \( \mathcal{P}_\Gamma^n = 0 \), the boundary conditions at \( \bar{\Gamma} \) are instead

\[
\theta^n_{\eta, \bar{\Gamma}} = \theta^{n, -n}_{\eta, \Gamma} = -\theta^n_{\eta, \bar{\Gamma}} = -\theta^{n, -n}_{\eta, \bar{\Gamma}},
\]

leading to spectrally-isolated quadruplets, e.g., in Fig. 5.2(f), (h) and (i). Since Kramers partners at \( \bar{\Gamma} \) (\( \bar{Z} \)) belong in opposite \( \eta \) subspaces (resp. the same \( \eta \) subspace), the interpolation describes an internal partner-switching within each quadruplet, resulting in an hourglass-like dispersion. The center of the hourglass is an unavoidable crossing [20] between opposite-\( \eta \) bands – this degeneracy is movable but unremovable. Finally, we remark that the interpolations distinguished by \( \mathcal{P}_\Gamma^n \) easily generalize beyond the minimal number of Wilson bands, e.g., compare Fig. 5.2(e) with (g).

Given that the Abelian polarization depends on the choice of spatial origin, [51] it may seem surprising that a single polarization invariant \( \mathcal{P}_\Gamma^n \) sufficiently indicates the GSHE;
indeed, each of the inequivalent inversion centers seems a reasonable choice for the spatial origin. In contrast, many other topologies are diagnosed by gauge-invariant differences in polarization. [51,75] Unlike generic polarizations, $P_\eta$ is invariant when a different inversion center is picked as origin, i.e., this globally shifts all $\theta \rightarrow \theta + \pi$ (e.g., Fig. 5.2(a) to (b)), which leads to $P_\eta / e \rightarrow P_\eta / e$ modulo $\mathbb{Z}$, since each glide subspace is even-dimensional.

One application regards the diagnosis of the GSHE from spatial-inversion ($I$) eigenvalues: we propose to multiply the $I$ eigenvalues of occupied bands in a single $\eta$ subspace, at the two inversion-invariant $k$ which project to $\tilde{\Gamma}$. This product being $+1$ ($-1$) then implies that $\mathcal{P}_\eta=0$ (resp. $=e/2$). In contrast, the usual quantum spin Hall effect (without glide symmetry) cannot [51, 70, 71] be formulated as an Abelian polarization, and a diagnosis would require all $\mathcal{I}$ eigenvalues in a two-torus. [54]

(ii) With trivial $\mathcal{P}_\eta$, the spectrally-isolated interpolations further subdivides into two distinct configurations, which are distinguished by an hourglass centered at $\theta = \pi$, e.g., contrast Fig. 5.2(a-b) with (c-d). This difference may be formalized by a $\mathbb{Z}_2$ topological invariant ($Q_0$), which we introduced in Chap. 4 as a quadruplet polarization.

**Connecting curves along the glide line $\tilde{X}\tilde{U}$**

While $\tilde{X}\tilde{U}$ and $\tilde{\Gamma}\tilde{Z}$ are both glide lines characterized by the same symmetries, the available sub-topologies on each line differ: while the two hourglass configurations (distinguished by a quadruplet polarization) are available sub-topologies on each line, the GSHE is only available along $\tilde{\Gamma}\tilde{Z}$. This difference arises because the same symmetries are represented differently on each line – the different projective representations are classified by the second cohomology group, as discussed in Sec. 5.3. For the purpose of topological classification, we need only extract one salient result from that Section: any Wilson band at $k = (\pi, k_z)$ and energy $\theta$ has simultaneously a ‘glide’ eigenvalue: $\lambda_x(k_z + \theta)$ in Eq. (5.5); here, ‘glide’ combines the ordinary glide reflection with parallel transport. We might ask if $\eta = \pm 1$
in $\lambda_x$ labels a meaningful division of the Wilson bands, i.e., do we once again have two non-interacting flavors of curves, as we had for $\tilde{\Gamma} \tilde{Z}$? The answer is affirmative if the Wilson bands are spectrally isolated, i.e., if all $n_{occ}$ Wilson bands lie strictly within an energy window of $2\pi$, for all $k_z \in [0, 2\pi)$. This isolation condition ensures at each $k_z$ that the energy difference $(\theta_i - \theta_j)$ between any two bands is strictly less than $2\pi$ — therefore there is no ambiguity in labelling each band by $\eta$ from Eq. (5.5). Conversely, this potential ambiguity is sufficient to rule out bands with spectral flow, as we now demonstrate.

Let us consider a hypothetical scenario with spectral flow (Fig. 5.3(c)), as would describe a GSHE. There is then a smooth interpolation between bands in one energy period to any band in the next, as illustrated by connecting black arrows in Fig. 5.3(c). As we interpolate $\theta \to \theta + 2\pi$ and $k_z \to k_z + 4\pi$, we of course return to the same eigenvector of $W$, and therefore the ‘glide’ eigenvalue must also return to itself. However, the energy-dependence leads to $\lambda_x \to -\lambda_x$. More generally for 4u number of occupied bands, $\theta \to \theta + 2\pi$ while $k_z \to k_z + 4u\pi$, leading to the same contradiction. Beside this argument, we furnish an alternative proof to rule out the GSHE in Sec. 4.1.4. We remark that the GSHE is perfectly consistent with the surface symmetries, [76] and it is only ruled out by a proper account of the bulk symmetries.

Returning to our classification, the tables inform us of the constraints due to time-reversal and spatial-inversion symmetries. The sum of this symmetry analysis is that our rules for the curves along $\tilde{X} \tilde{U}$ are completely identical to that along $\tilde{\Gamma} \tilde{Z}$, assuming that bands are spectrally isolated. We thus conclude that there are two hourglass-type interpolations (Fig. 5.3(a-b)), which are distinguished by a second quadruplet polarization ($Q_x$).
Connecting curves along the mirror line $\tilde{\Gamma}\tilde{X}$

(a) Curves divide into two non-interacting flavors (red solid and red dashed), corresponding to $\tilde{M}_z = \pm i$ subspaces.

(b) At both boundaries ($\tilde{\Gamma}$ and $\tilde{X}$), each red solid curve is degenerate with a red dashed curve.

(c) At any point along $\tilde{\Gamma}\tilde{X}$, $[\theta, \text{red solid}] \leftrightarrow [-\theta, \text{red dashed}]$.

These rules allow for mirror-Chern topologies, [34] where $\tilde{M}_z = \pm i$ subspaces have opposite chirality. The allowed mirror Chern numbers ($C_e$) depend on our last rule:

(d) Curves must match continuously at $\tilde{\Gamma}$ and $\tilde{X}$.

This last rule imposes a consistency condition with the sub-topologies at $\tilde{\Gamma}\tilde{Z}$ and $\tilde{X}\tilde{U}$: $C_e$ is odd (even) if and only if $\mathcal{P}_\Gamma^{\text{re}} = e/2$ (resp. $\mathcal{P}_\Gamma^{\text{re}} = 0$), as illustrated in Fig. 5.4(a-c) (resp. 5.4(d-f)).

To demonstrate our claim, we rely on a ‘Fermi-level’ criterion to determine the parity of $C_e$: decide arbitrarily on a Fermi energy, then count the parity of $M_z = +i$ bands at the Fermi level – both parities equal. Counting here is done along the full circle $\tilde{X}\tilde{\Gamma}\tilde{X}$. Since time reversal relates $M_z = \pm i$ bands at opposite momentum, a modified counting rule applies to the half-circle $\tilde{\Gamma}\tilde{X}$: (i) away from the end points, count the parity of every band,
in both $\bar{M}_z = \pm i$ subspaces. (ii) To avoid overcounting at the end points, every Kramers subspace at the Fermi level counts as one. Summing (i) and (ii) produces the parity of $\mathcal{C}_e$.

Supposing the Fermi energy to be zero, we would be interested in the number of zero-energy Kramers subspaces (ZEKS) at the end points. The number of ZEKS at $\tilde{\Gamma}$ has been established in Sec. 5.2.2: odd if $\mathcal{P}^{\eta}_{\tilde{\Gamma}} = e/2$, and even if $\mathcal{P}^{\eta}_{\tilde{\Gamma}} = 0$. Moreover, this parity alone is decisive, because every other contribution has even parity, as we now show. First at $\tilde{X}$. Given that the only sub-topologies at $\tilde{X}\tilde{U}$ are hourglasses, there are generically no ZEKS at $\tilde{X}$ (Fig. 5.4(a) and (c-f)), though in fine-tuned situations (Fig. 5.4(b)) there might be an even number. Away from the end points, any intersection comes in particle-hole-symmetric pairs (e.g., Fig. 5.4(c), (e-f)).

![Figure 5.4: Possible Wilson spectra along $\tilde{\Gamma}\tilde{X}$](image)

Figure 5.4: Possible Wilson spectra along $\tilde{\Gamma}\tilde{X}$ (a-c) With nontrivial glide polarization ($\mathcal{P}^{\eta}_{\tilde{\Gamma}}$), the mirror Chern numbers ($\mathcal{C}_e$) are respectively $-1, +1$ and $-3$. (d-f) With trivial $\mathcal{P}^{\eta}_{\tilde{\Gamma}}$, $\mathcal{C}_e$ equals $0, -2$ and $-4$ respectively.

**Connecting curves along the mirror line $\tilde{Z}\tilde{U}$**

(a) Each red, solid curve ($\bar{M}_z = + i$) is degenerate with a red, dashed curve ($\bar{M}_z = - i$). Doublet curves cannot cross, and must be symmetric under $\theta \rightarrow -\theta$.

(b) The curve-matching conditions at $\tilde{Z}$ and $\tilde{U}$ again imposes consistency requirements.
These rules are stringent enough to uniquely specify the interpolation along $\tilde{Z}\tilde{U}$, given the sub-topologies at $\tilde{\Gamma}\tilde{Z}$ (specified by $P_{\tilde{\eta}}$, $Q_0$) and at $\tilde{X}\tilde{U}$ ($Q_{\pi}$). Alternatively stated, there are no additional invariants in this already-complete classification. To justify our claim, first consider $P_{\tilde{\eta}} = e/2$, such that doublets at $\tilde{U}$ are matched with ‘handles’ of hourglasses (along $\tilde{U}\tilde{X}$), while doublets at $\tilde{Z}$ connect to cusps of a zigzag (along $\tilde{Z}\tilde{\Gamma}$). There is then only one type of interpolation illustrated in Fig. 5.5(a-c). If $P_{\tilde{\eta}} = 0$, we have hourglasses on both ‘sides’. If on one ‘side’ an hourglass is centered at $\theta = \pi$, while there is no $\pi$-hourglass on the other ‘side’ (i.e., $Q_0 \neq Q_{\pi}$), the unique interpolation is shown in Fig. 5.5(d-e): red doublets connect the ‘upper handle’ of one hourglass to the ‘lower handle’ of another, in a generalized zigzag pattern. A brief remark here is in order: when viewed individually along any straight line (e.g., $\tilde{\Gamma}\tilde{Z}$ or $\tilde{Z}\tilde{U}$), bands are clearly spectrally isolated; however, when viewed along a bent line ($\tilde{\Gamma}\tilde{Z}\tilde{U}\tilde{X}$), the bands exhibit spectral flow. In all other cases for $P_{\tilde{\eta}}$, $Q_0$ and $Q_{\pi}$, bands along $\tilde{\Gamma}\tilde{Z}\tilde{U}\tilde{X}$ separate into spectrally-isolated quadruplets, as in Fig. 5.5(f).

Figure 5.5: Possible Wilson spectra along $\tilde{Z}\tilde{U}$.

5.2.3 Na$_3$Bi under pressure is a glide spin Hall insulator

Our classification is predictive of the topological nature of Dirac-semimetallic Na$_3$Bi, [69] which has the same space group as KHgX. In an earlier work, [69] we have shown that Na$_3$Bi is parity-inverted and $Z_2$-nontrivial [54] in the $k_z=0$ plane; the $Z_2$ topology implies
that the mirror Chern number ($C_e$) is odd. By our classification, this implies a GSHE in the $k_x=0$ plane, if Na$_3$Bi were insulating in that plane. However, the three-fold rotational symmetry along $\Gamma - Z$ protects Dirac crossings between conduction and valence bands; [69] to realize the GSHE, this three-fold symmetry must be broken, while preserving spatial-inversion and $Pma2$ symmetries – one experimentally feasible option is to apply pressure in $\vec{x}$, assuming such pressure does not induce a structural phase transition. To support our hypothesis, we evaluated the Wilson loop of pressured Na$_3$Bi in Fig. 5.6; the zigzag connectivity along $\tilde{\Gamma} \tilde{Z}$ ($\tilde{\Gamma} \tilde{X}$) confirms the GSHE (resp. that $C_e = 1$).

![Figure 5.6: Wilson-loop spectrum of pressured Na$_3$Bi.](image)

### 5.3 Extended group of Wilsonian symmetries and group cohomology in band insulators

Symmetry operations normally describe space-time transformations; such symmetries and their groups are referred to as ordinary. Here, we encounter certain ‘symmetries’ of the Wilson loop which additionally induce parallel transport; we call them W-symmetries to distinguish them from the ordinary symmetries. In this Section, we identify the relevant W-symmetries, and show their corresponding group ($G_{\pi,kz}$) to be an extension of the ordinary group ($G_s$), which correspond purely to space-time transformations. The inequivalent extensions are classified by the second cohomology group, which we introduce here.
W-symmetries are a special type of constraints on the Wilson loop. As exemplified in Eq. (5.3) and (5.4), constraints ($\mathcal{R}$) on a Wilson loop ($\mathcal{W}$) map $\mathcal{W}$ to itself, up to a reversal in orientation:

$$\mathcal{R} \mathcal{W} \mathcal{R}^{-1} = \mathcal{W}^\pm 1,$$

where $\mathcal{W}^{-1}$ is the inverse of $\mathcal{W}$; all $\mathcal{R}$ satisfying this equation are defined as elements in the group of the Wilson loop. A trivial example of $\mathcal{R}$ would be the Wilson loop itself; $\mathcal{R}$ may also represent a space-time transformation, as exemplified by a $2\pi$ real-space rotation ($\vec{E}$). Particularizing to our context, we let $k_y \in (-\pi, \pi)$ parametrize the non-contractible momentum loop, and choose the convention that $\mathcal{W}$ ($\mathcal{W}^{-1}$) effects parallel transport in the positive orientation: $+2\pi \vec{y}$ (resp. in the reversed orientation: $-2\pi \vec{y}$).

W-symmetries arise as constraints if a space-time transformation exists that maps: $k_y \rightarrow \pm k_y + \pi$. Our first example of a W-symmetry has been introduced in Sec. 5.2.1, namely that the glide reflection ($\vec{M}_x$) maps: $(k_y, k_z) \rightarrow (k_y + \pi, k_z)$, for any $k_z$ along $k_x = \pi$. Consequently,

$$\vec{M}_x \mathcal{W}_{-\pi}(\pi, k_z) \vec{M}_x^{-1} = \mathcal{W}_0(\pi, k_z),$$

where we have indicated the base point of the parameter loop as a subscript of $\mathcal{W}$, i.e., $\mathcal{W}_{k_y}$ induces parallel transport from $(\vec{k}_y, \pi, k_z)$ to $(\vec{k}_y + 2\pi, \pi, k_z)$. As it stands, Eq. (5.10) is not a constraint as defined in Eq. (5.9). Progress is made further parallel-transporting the occupied space by $-\pi \vec{y}$, such that we return to the initial momentum: $(k_y, \pi, k_z)$. This motivates the definition of a W-glide symmetry ($\vec{M}_x$) which combines the glide reflection ($\vec{M}_x$) with parallel transport across half a reciprocal period – then by our construction, $\vec{M}_x$ is an element in the group ($G_{\pi, k_z}$) of $\mathcal{W}_{-\pi}(\pi, k_z)$). To be precise, let us define the Wilson line $\mathcal{W}_{-\pi+0}$ to represent a parallel transport from $(0, \pi, k_z)$ to $(-\pi, \pi, k_z)$, then

$$\vec{M}_x \mathcal{W}_{-\pi} \vec{M}_x^{-1} = \mathcal{W}_{-\pi}, \text{ with } \vec{M}_x = \mathcal{W}_{-\pi+0} \vec{M}_x.$$
The W-glide squares as:

\[ \tilde{M}_x^2 = \bar{E} t(\bar{z}) W_{-\pi}^{-1}, \]  

(5.12)

which may be understood loosely as follows: the glide component of the W-operation squares as a \(2\pi\) rotation (\(\bar{E}\)) with a lattice translation (\(t(\bar{z})\)), while the transport component squares as a full-period transport (\(W^{-1}\)); we defer the detailed derivations of Eq. (5.10)-(5.12) to App. 5.4.4. For a Wilson band with energy \(\theta(k_z)\), Eq. (5.12) implies the corresponding W-glide eigenvalue depends on the sum of energy and momentum, as in Eq. (5.5). Our construction of \(\tilde{M}_x\) is a quasimomentum-analog of the non-symmorphic extension of point groups. For example, the glide reflection (\(\tilde{M}_x\)) combines a reflection with half a real-lattice translation – \(\tilde{M}_x^2\) thus squares to a full lattice translation, which necessitates extending the point group by the group of translations. Here, we have further combined \(\tilde{M}_x\) with half a reciprocal-lattice translation, thus necessitating a further extension by Wilson loops.

Our second example of a W-symmetry (\(T\)) belongs in the groups of \(W(\tilde{X})\) and \(W(\tilde{U})\), which correspond to the two time-reversal-invariant \(k_n\) along \(k_x = \pi\) (recall Fig. 4.2); since both groups are isomorphic, we use a common label: \(G_{\tilde{X}}\). \(T\) combines time reversal (\(T\)) with parallel transport over a half period, as follows from time reversal mapping: \((k_y, \pi, \bar{k}_z) \rightarrow (-k_y, -\pi, -\bar{k}_z) = (-k_y + \pi, \pi, \bar{k}_z) - \bar{b}_2 - 2\bar{k}_z \bar{z}\) for \(\bar{k}_z \in \{0, \pi\}\), as illustrated in Fig. 4.7(c). Consequently,

\[ T W_{-\pi} T^{-1} \overset{\bar{k}_z}{=} W_{r,2\pi}, \]  

(5.13)

where \(W_{r,2\pi}\) denotes the reverse-oriented Wilson loop with base point \(2\pi\), and \(\bar{k}_z\) indicates that this equality holds for \(k_n \in \{\tilde{X}, \tilde{U}\}\). Eq. (5.13) motivates combining \(T\) with a half-period transport, such that

\[ T W_{-\pi} T^{-1} \overset{\bar{k}_z}{=} W_{-\pi}^{-1}, \quad \text{with} \quad T \overset{\bar{k}_z}{=} W_{-\pi=0} T. \]  

(5.14)

To complete the Wilsonian algebra,

\[ T^2 \overset{\bar{k}_z}{=} \bar{E}, \quad \tilde{M}_x T \overset{\bar{k}_z}{=} T \tilde{M}_x W_{-\pi}, \]  

(5.15)
as derived in App. 5.4.4. This result, together with Eq. (5.12), may be compared with the ordinary algebra of space-time transformations:

\[ \bar{M}_x^2 = \bar{E} t(\vec{z}), \quad T^2 \equiv \bar{E}, \quad \bar{M}_x T \equiv T \bar{M}_x, \quad (5.16) \]

as would apply to the surface bands at any time-reversal-invariant \( \vec{k} \). Both algebras are identical modulo factors of \( \mathcal{W} \) and its inverse; from hereon, \( \mathcal{W}(\vec{k})_\pi = \mathcal{W} \). We emphasize that the same edge symmetries are represented differently in the surface Hamiltonion \( H_s \) and in \( \mathcal{W} \) – this difference originates from the out-of-surface translational symmetry \( (t_\perp) \), which distinguishes the bulk wavevectors \( k_y \) from \( k_y + \pi \).

To further describe this difference group-theoretically, let us define \( G_s \) as a symmorphic group for a spinless particle. Its generators are the glideless reflection \( (M_x) \) and time reversal \( (T) \), which satisfy

\[ M_x^2 = I, \quad T^2 = I, \quad [M_x, T] = 0. \quad (5.17) \]

The algebra of Eq. (5.16) describes a well-known, non-symmorphic extension of \( G_s \) for spinful particles; we propose that Eq. (5.12) and (5.15) describe a further extension of Eq. (5.16) by reciprocal translations. That is, \( \tilde{G}_X \) is an extension of \( G_s \) by \( \mathcal{N} \), where \( \mathcal{N} \) is generated by \( \bar{E}, \mathcal{W} \) and \( t(\vec{z}) \); for an introduction to group extensions and their application to our problem, we refer to the interested reader to App. 5.6. There exists another extension (inequivalent to \( \tilde{G}_X \)) which applies to our crystal; in Sec. 5.2.2, we further show that inequivalent extensions lead to different topologies for the Wilson bands. This implication motivates a precise definition of equivalence: two extensions (of \( G_s \) by \( \mathcal{N} \)) are equivalent if they correspond to the same element in the second cohomology group \( H^2(G_s, \mathcal{N}) \). The elements of this Abelian group are equivalence class of factor systems \( \{C_{f,g}\} \), defined by

\[ \hat{f} \hat{g} = C_{f,g} \hat{f} \hat{g} \quad \text{for} \quad f, g \in G_s, \quad C_{f,g} \in \mathcal{N}. \quad (5.18) \]

Here, we distinguish between elements (e.g., \( \{f = M_x, g = T\} \)) of \( G_s \), and their corresponding projective representations \( \{\hat{f} = \hat{M}_x, \hat{g} = \hat{T}\} \) in the extension by \( \mathcal{N} \); different elements of
\( H^2(G_s, \mathcal{N}) \) correspond to different projective representations of \( G_s \). Factor systems satisfy a generalized two-cocycle condition:

\[
C^{-1}_{fg,h} C^{-1}_{f,g} \sigma_f(C_{g,h}) C_{f,gh} = I, \tag{5.19}
\]

which follows from demanding that \( \hat{f} \hat{g} \hat{h} \) is associative. Here, \( \sigma_f \) is an automorphism of \( \mathcal{N} \):

\[
\sigma_f(W^n) = \hat{f} W^n \hat{f}^{-1} = W^{\gamma(f)n} \text{ with } \gamma(f) = \pm 1, \tag{5.20}
\]

e.g., \( \gamma(\hat{M}_x) = +1 \) follows from Eq. (5.11), and \( \gamma(T) = -1 \) from Eq. (5.14). Two factor systems are equivalent if they are related by a gauge transformation

\[
\hat{g} \rightarrow \hat{g} W^{n(g)} \text{ with } n(g) \in \mathbb{Z}. \tag{5.21}
\]

In either gauge for \( \hat{g} \), the same constraint is imposed on \( W \), since

\[
\hat{g} W^{n(g)} W (\hat{g} W^{n(g)})^{-1} = \hat{g} W \hat{g}^{-1}. \tag{5.22}
\]

To exemplify an extension that is inequivalent to \( G_\check{\chi} \), let us consider the group \( (G_r) \) of \( W(\check{\Gamma}) \); \( G_r \) is isomorphic to the group of \( W(\check{Z}) \); recall that both \( \check{\Gamma} \) and \( \check{Z} \) are time-reversal-invariant \( k \), along \( k_x = 0 \). \( k_x = 0 \) labels a glide line in the 010-surface BZ, which guarantees the \( k_x = 0 \) plane (in the bulk BZ) is mapped to itself under the glide \( \check{M}_x \); the same could be said for \( k_x = \pi \). However, unlike \( k_x = \pi \), \( \check{M}_x \) belongs to the group of any bulk wavevector in the \( k_x = 0 \) plane, and therefore

\[
\check{M}_x W(\check{\Gamma}) \check{M}_x^{-1} = W(\check{\Gamma}) \tag{5.23}
\]

with \( \check{M}_x \) an ordinary space-time symmetry, i.e., \( \check{M}_x \) does not encode parallel transport. Consequently, this element of \( G_r \) satisfies the ordinary algebra in Eq. (5.16); by an analogous derivation, the time reversal element in \( G_r \) is also ordinary. It is also apparent why \( G_\check{\chi} \) and \( G_r \) are inequivalent extensions: there exists no gauge transformation that relates their factor systems, e.g.,

\[
\check{M}_x T = T \check{M}_x W \rightarrow \check{M}_x T = T \check{M}_x W^{1+2n(T)}. \tag{5.24}
\]
ensures that the parity of the exponent is gauge-invariantly odd. $G_\tilde{X}$ is then an example of an intrinsically projective representation, wherein its factor system can never be ‘lifted’ no matter the gauge choice.

Finally, we remark that this Section does not exhaust all elements in $G_\tilde{X}$ or $G_\tilde{I}$; our treatment here minimally conveys their group structures. A complete treatment of $G_\tilde{X}$ is offered in App. 5.4.4, where we also derive the above algebraic relations in greater detail.

5.4 Symmetries of the Wilson loop

The goal of this Appendix is to derive how symmetries of the Wilson loop are represented, and their implications for the ‘rules of the curves’, as summarized in Tab. 5.2 and 5.3. After introducing some notations in App. 5.4.1, we consider in App. 5.4.2 the effect of spatial symmetries on the Wilson loop, with particular emphasis on glide symmetry. We then generalize our discussion to space-time symmetries in Sec. 5.4.3. These first sections apply only to symmetries along $\tilde{X} \tilde{I} \tilde{Z} \tilde{U}$, and the symmetry representations are shown to be ordinary, i.e., they do not encode quasimomentum transport; their well-known algebra is summarized as:

\[
\begin{align*}
\bar{M}_x^2 &= \bar{E} \ t(c\vec{z}), \quad (T \bar{M}_x)^2 = I, \\
\bar{M}_x T \bar{M}_x &= \bar{E} \ t(c\vec{z}) \ T \bar{M}_x \bar{M}_x, \quad T^2 = (TT)^2 = \bar{E}, \\
\bar{M}_x IT &= t(c\vec{z}) IT \bar{M}_x, \quad \bar{M}_x T = T \bar{M}_x. \\
\end{align*}
\]

In App. 5.4.4, we move on to derive the projective representations which apply along $\tilde{X} \tilde{U}$. 
5.4.1 Notations for the Wilson loop

Consider the parallel transport of occupied bands along the non-contractible loops of Sec. 5.1.1. In the orbital basis, such transport is represented by the Wilson-loop operator: \[ \hat{W}(k) = V(2\pi \vec{y}) \prod_{k_y} P(k_y, k_i). \] (5.26)

Here, we have discretized the momentum as \( k_y = 2\pi m/N_y \) for integer \( m = 1, \ldots, N_y \), and \( (\pi \leftarrow -\pi) \) indicates that the product of projections is path-ordered. Recall our the unconventional ordering: \( k = (k_y, k_x, k_z) = (k_y, k_i) \). In the basis of \( n_{\text{occ}} \) occupied bands, this same parallel transport is represented by an \( n_{\text{occ}} \times n_{\text{occ}} \) matrix:

\[
[\hat{W}(k)]_{ij} = \langle u_i, (-\pi, k_i) \| \hat{W}(k) \| u_j, (-\pi, k_i) \rangle.
\] (5.27)

While \( \hat{W} \) depends on the choice of gauge for \( |u_{n, -\pi, k_i}\rangle \), its eigenspectrum does not. In the limit of large \( N_y \), \( \hat{W} \) becomes unitary and its full eigenspectrum comprises the unimodular eigenvalues of \( \hat{W} \), which we label by \( \exp[i\theta_{n,k_i}] \) with \( n = 1, \ldots, n_{\text{occ}} \). Denoting the eigenvalues of \( \hat{y}_\perp \hat{P}_\perp \) as \( y_{n,k_i} \), the two spectra are related as \( y_{n,k_i} = \theta_{n,k_i}/2\pi \) modulo one. [51]

5.4.2 Effect of spatial symmetries of the 010 surface

Let us describe the effect of symmetry on the spectrum of \( \hat{W} \). First, we consider a generic spatial symmetry \( g_\delta \), which transforms real-space coordinates as \( r \rightarrow D_g r + \delta \). From Eq. (1.26), we obtain the constraints on the projections as

\[
\hat{g}_\delta(k) P(k) \hat{g}_\delta(k)^{-1} = P(D_g k).
\] (5.28)

The constraints on \( \hat{W} \) arise only from a subset of the symmetries that either (i) map one loop parametrized by \( k_i \) to another loop at a different \( k_i \), or (ii) map a loop to itself. We say that two loops are mapped to each other even if the mapping reverses the loop orientation, or translates the base point of the loop. We exemplify these statements with the symmetries of the 010 surface, which satisfy either (i) or (ii). All spatial symmetries
of the 010 surface preserve the $y$ coordinate, and transforms the surface coordinates as 
\[ (x, z)^t \rightarrow D_\parallel^g(x, z)^t + (\delta x, \delta z) \] with \( \delta_\parallel = \delta x \vec{x} + \delta z \vec{z} \); the occupied-band projections are likewise constrained as

\[
\hat{g}_\delta(k_y, k_n) P(k_y, k_n) \hat{g}_\delta(k_y, k_n)^{-1} = P( k_y, D_\parallel^g k_n ),
\]

and Eq. (1.29) particularizes to

\[
\hat{g}_\delta(\pi, k_n) V(2 \pi \vec{y}) = e^{-i2\pi \vec{y} \cdot \delta_\parallel} V(2 \pi \vec{y}) \hat{g}_\delta(\pi, k_n) = V(2 \pi \vec{y}) \hat{g}_\delta(\pi, k_n). \tag{5.30}
\]

Applying Eq. (5.26), (5.29) and (5.30),

\[
\hat{g}_\delta(\pi, k_n) \hat{W}(k_n) \hat{g}_\delta(\pi, k_n)^{-1} = \hat{W}( D_\parallel^g k_n ). \tag{5.31}
\]

Then by inserting in Eq. (5.31) a complete set of states at momentum \( k = (\pi, k_n) \), and further applying Eq. (1.27) and (5.27),

\[
\hat{g}_\delta(\pi, k_n) \hat{W}(k_n) \hat{g}_\delta(\pi, k_n)^{-1} = \hat{W}( D_\parallel^g k_n ). \tag{5.32}
\]

Let us exemplify this discussion with the glide reflection which transforms spatial coordinates as \((x, y, z) \rightarrow (-x, y, z + 1/2)\). Following the notation in the main text, we define \( \bar{M}_x \equiv M_{x,z/2} \) with \( g = M_x \) a reflection and \( \delta = \vec{z}/2 \) a fractional translation. This symmetry acts on Bloch waves as \( \hat{M}_x(k) = e^{-ik_z/2} U_{\delta z} \) (from Eq. (1.15)), with \( U_{\delta z}^2 = -I \) representing a \( 2\pi \) rotation. Eq. (5.32) assumes the form

\[
\hat{M}_x(\pi, k_n) \hat{W}(k_x, k_z) \hat{M}_x(\pi, k_n)^{-1} = \hat{W}( -k_x, k_z ). \tag{5.33}
\]

Since \( \bar{M}_x \) transforms momentum as \( k \rightarrow (k_y, -k_x, k_z) \), it belongs in the group of any wavevector with \( k_x = 0 \). Indeed, \( [\bar{M}_x(\pi, 0, k_z), \hat{W}(0, k_z)] = 0 \), and each Wilson band may be labelled by an eigenvalue of \( \bar{M}_x \), which again falls into either branch of \( \pm i \exp(-ik_z/2), \)
as we now show:

\[
[M_x(k_1)]^2_{mn} = e^{-i k_z} \sum_{n_{occ}} \langle u_{m,k_1} | U_{\bar{M}_x} u_{a,k_1} \rangle \langle u_{a,k_1} | U_{\bar{M}_x} u_{n,k_1} \rangle = e^{-i k_z} \sum_{a=1}^{n_{tot}} \langle u_{m,k_1} | U_{\bar{M}_x} u_{a,k_1} \rangle \langle u_{a,k_1} | U_{\bar{M}_x} u_{n,k_1} \rangle = e^{-i k_z} \langle u_{m,k_1} | (U_{\bar{M}_x})^2 | u_{n,k_1} \rangle = e^{-i k_z} \delta_{mn}.
\]

Here, \( k_1 \equiv (-\pi, 0, k_z) \); in the second equality, we denote \( n_{tot} \) as the total number of bands, and applied that the symmetry representations are block-diagonal with respect to the occupied and empty subspaces; the completeness relation was used in the third, and \((U_{\bar{M}_x})^2 = -I\) represents a \(2\pi\) rotation.

5.4.3 Effect of space-time symmetries

Suppose our Hamiltonian is symmetric under a space-time transformation \( T_{g\delta} \). Following Eq. (1.34), the occupied-band projection is constrained as

\[
\hat{T}_{g\delta}(k) P(k) \hat{T}_{g\delta}(k) = P(-D_g k).
\]

This, in combination with Eq. (1.38) and (5.26), implies

\[
\hat{T}_{g\delta}(-\pi, k_n) \hat{W}(k_n) \hat{T}_{g\delta}(-\pi, k_n)^{-1} = e^{i D_g (2\pi \hat{y})} V(-D_g (2\pi \hat{y})) \prod_{k_y} P(-D_g k).
\]

In the next few subsections, we particularize to a few examples of \( T_{g\delta} \) that are relevant to the topology of our space group.

Effect of space-time inversion symmetry

The space-time inversion symmetry \((TT)\) maps \((x, y, z, t) \rightarrow -(x, y, z, t)\). Let us show how this results in a ‘particle-hole’ symmetric spectrum for \( W \), i.e., the eigenvalues form complex-conjugate pairs. Inserting \( D_g = -I \) and \( \delta = 0 \) in Eq. (5.36),

\[
\hat{T}_x(-\pi, k_n) \hat{W}(k_n) \hat{T}_x(-\pi, k_n)^{-1} = \hat{W}(k_n).
\]
Then by inserting in Eq. (5.37) a complete set of states at momentum $k = (-\pi, k_n)$, and applying the definitions (5.27) and (1.36),

$$\hat{T}_x(-\pi, k_n) W(k_n) \hat{T}_x(-\pi, k_n)^{-1} = W(k_n).$$

(5.38)

Thus if an eigensolution exists with eigenvalue $\exp[i\theta(k_n)]$, there exists a partner solution with the complex-conjugate eigenvalue $\exp[-i\theta(k_n)]$. After proving that $\hat{T}_x^2 = -I$, we would conclude that these two solutions are mutually orthogonal. The proof is elementary:

$$[\hat{T}_x^2(k)]_{mn} = \sum_{a=1}^{n_{oc}} \langle u_m, k | \hat{T}_x(k) | u_{a, k} \rangle \langle u_{a, k} | \hat{T}_x(k) | u_n, k \rangle$$

$$= \sum_{a=1}^{n_{tot}} \langle u_m, k | \hat{T}_x(k) | u_{a, k} \rangle \langle u_{a, k} | \hat{T}_x(k) | u_n, k \rangle$$

$$= \langle u_m, k | \hat{T}_x(k) \rangle^2 | u_n, k \rangle = \langle u_m, k | U_{IT} U^*_{IT} | u_n, k \rangle = -\langle u_m, k | u_n, k \rangle = -\delta_{mn}.$$  

(5.39)

In the second equality, we denote $n_{tot}$ as the total number of bands, and applied that the symmetry representations are block-diagonal with respect to the occupied and empty subspaces; the completeness relation was used in the third, and $U_{IT} U^*_{IT} = -I$ follows because $(TT)^2$ is a $2\pi$ rotation.

**Effect of time reversal with a spatial glide-reflection**

The symmetry $TM_x$ maps $(x, y, z, t) \rightarrow (-x, y, z + c/2, -t)$. Particularizing Eq. (5.36) to this symmetry,

$$\hat{T}_{M_x}(-\pi, k_x, k_z) \tilde{W}(k_x, k_z) \hat{T}_{M_x}(-\pi, k_x, k_z)^{-1} = \tilde{W}_x(k_x, -k_z),$$

(5.40)

where the reversed Wilson-loop operator is defined in Eq. (5.50). An equivalent expression in the occupied-band basis is

$$\hat{T}_{M_x}(-\pi, k_x, k_z) W(k_x, k_z) \hat{T}_{M_x}(-\pi, k_x, k_z)^{-1} = W(k_x, -k_z)^{-1},$$

(5.41)

where the inverse Wilson loop has been defined in Eq. (5.49); it is worth clarifying that

$$\hat{T}_{M_x}(-\pi, k_x, k_z)_{mn} = \langle u_m, (\pi, k_x, -k_z) | \hat{T}_{M_x} | u_n, (-\pi, k_x, k_z) \rangle$$

(5.42)
with
\[ |u_{m,(\pi,k_z,-k_z)}\rangle = V(-2\pi\tilde{y}) |u_{m,(-\pi,k_z,-k_z)}\rangle. \] (5.43)

We now focus on \( k_z = \tilde{k}_z \) satisfying \( \tilde{k}_z = -\tilde{k}_z \) modulo \( 2\pi \), where the symmetry maps any Wilson loop to itself, with a reversal of orientation. Eq. (5.41) then particularizes to
\[ \tilde{T}_{\delta x}(k_1,k_1) \mathcal{W}(k_x,\tilde{k}_z) \tilde{T}_{\delta x}(k_1,k_1)^{-1} = \mathcal{W}(k_x,\tilde{k}_z)^{-1}, \text{ with } k_1 = (-\pi,k_x,\tilde{k}_z), \] (5.44)
and \( \tilde{T}_{\delta x}(k_1,k_1) \) defined in Eq. (1.36). Let us prove that
\[ \tilde{T}_{\delta x}(k_1,k_1)^2 = \begin{cases} +I, & \tilde{k}_z = 0 \\ -I, & \tilde{k}_z = \pi, \end{cases} \] (5.45)
from which we may deduce a Kramers-like degeneracy in the spectrum of \( \mathcal{W}(k_x,k_z = \pi) \).

\[ \left[ \tilde{T}_{\delta x}(k_1,k_1)^2 \right]_{mn} \]
\[ = \sum_{a=1}^{n_{occ}} \langle u_{m,k_1} | V(2\pi\tilde{y} - 2\tilde{k}_z \tilde{z}) \tilde{T}_{\delta x}(k_1) | u_{a,k_1} \rangle \langle u_{a,k_1} | V(2\pi\tilde{y} - 2\tilde{k}_z \tilde{z}) \tilde{T}_{\delta x}(k_1) | u_{n,k_1} \rangle \]
\[ = \sum_{a=1}^{n_{occ}} \langle u_{m,k_1} | V(2\pi\tilde{y} - 2\tilde{k}_z \tilde{z}) \tilde{T}_{\delta x}(k_1) | u_{a,k_1} \rangle \langle u_{a,k_1} | V(2\pi\tilde{y} - 2\tilde{k}_z \tilde{z}) \tilde{T}_{\delta x}(k_1) | u_{n,k_1} \rangle \]
\[ = \langle u_{m,k_1} | V(2\pi\tilde{y} - 2\tilde{k}_z \tilde{z}) \tilde{T}_{\delta x}(k_1) V(2\pi\tilde{y} - 2\tilde{k}_z \tilde{z}) \tilde{T}_{\delta x}(k_1) | u_{n,k_1} \rangle \]
\[ = \langle u_{m,k_1} | U_{\delta x} U_{\delta x}^* | u_{n,k_1} \rangle = e^{-ik_z} \langle u_{m,k_1} | U_{\delta x} | u_{n,k_1} \rangle = e^{-ik_z} \delta_{mn}. \] (5.46)

In the second equality, we applied that the symmetry representations are block-diagonal with respect to the occupied and empty subspaces; the completeness relation was used in the third, Eq. (1.38) in the fourth, and \( U_{\delta x} U_{\delta x}^* = +I \) represents the point-group relation that \( (TM_x)^2 \) is just the identity transformation; cf. our discussion in App. 1.2.

**Effect of time-reversal symmetry**

Let us particularize the discussion in Sec. 1.3 by letting \( g_\delta \) in \( Tg_\delta \) be the trivial transformation. Time reversal acts on Bloch waves as the antiunitary operator \( \hat{T} = U_T K \), where
$U_T U_T^* = -I$ corresponds to a $2\pi$ rotation of a half-integer spin. We obtain from Eq. (5.36) that

$$\hat{T} \hat{W}(k) \hat{T}^{-1} = V(\pm 2\pi \vec{y}) \prod_{k_y} P(-k) = V(\pm 2\pi \vec{y}) \prod_{k_y} P(k_y, -k_y) = \hat{W}_{\tau}(-k),$$

where the last equality defines the reverse-oriented Wilson loop. Equivalently,

$$\hat{T}(\mp, k) W(k) \hat{T}(\pm, k)^{-1} = W(-k)^{-1},$$

where the inverse Wilson loop may be expressed as

$$[W(k)]^{-1}_{ij} = [W(k)]^*_{ji} = \langle u_{i,(\mp,k)} | \hat{W}_{\tau}(k) | u_{j,(\pm,k)} \rangle,$$

with

$$|u_{j,(\mp,k)}\rangle = V(\pm 2\pi \vec{y}) |u_{j,(\pm,k)}\rangle.$$

Time reversal thus maps $\exp[i\theta_{k_z}] \rightarrow \exp[i\theta_{-k_z}]$. Following an exercise similar to the previous section, one may derive a Kramers degeneracy where $k_q = -k_q$ (up to a reciprocal vector).

### 5.4.4 Extended group algebra of the W-symmetries along $\tilde{X}\tilde{U}$

Our aim is to derive the algebra of the group $(G_{\pi,k_z})$ of $W(\pi,k_z)$, which we introduced in Sec. 5.3. $k_z = 0$ and $\pi$ mark the time-reversal invariant $k$, namely, $\tilde{X}$ and $\tilde{U}$. Here, $G_{\tilde{X}} \cong G_{\tilde{U}}$ has the elements: $2\pi$ rotation ($\bar{E}$), the lattice translation $t(\vec{z})$, the Wilson loop ($W$), and analogs of time reversal ($T$), spatial inversion ($I$) and glide reflection ($\bar{M}_x$) that additionally encode parallel transport; the latter three are referred to as W-symmetries. In addition to deriving the algebraic relations in Eq. (5.11) and (5.15), we also show here that:

(a) The combination of time reversal, spatial glide and parallel transport is an element $T_{\tilde{M}_z}$ with the algebra:

$$T_{\tilde{M}_z} W T_{\tilde{M}_z}^{-1} = W^{-1}, \quad \text{with} \quad T_{\tilde{M}_z}^2 = I$$

and

$$\bar{M}_x T_{\tilde{M}_z} = \bar{E} \ t(\vec{z}) \ T_{\tilde{M}_z} \bar{M}_x \ W.$$  

(5.51)
(b) The space-time inversion symmetry acts in the ordinary manner:

\[ \mathcal{T}_I \mathcal{W} \mathcal{T}_I^{-1} = \mathcal{W}, \quad \mathcal{T}_I^2 = \bar{E}, \quad \bar{M}_x \mathcal{T}_I = t(\hat{z}) \mathcal{T}_I \bar{M}_x. \]  

(5.52)

The algebra that we derive here extends the ordinary algebra of space-time transformations, which we showed in Eq. (5.25). For time-reversal-variant \( k_q \) along the same glide line, \( G_{\pi,kz} \) is a subgroup of \( G_X \), and is instead generated by \( \bar{E}, t(R), \mathcal{W}, \bar{M}_x, \mathcal{M}_z \) and \( \mathcal{T}_I \). Therefore, Eq. (5.11), (5.51) and (5.52) (but not Eq. (5.15)) would apply to \( G_{\pi,kz} \) \( (k_z \notin \{0, \pi\}) \). Eq. (5.11), (5.51), (5.52) and (5.15) are respectively derived in App. 5.4.4, 5.4.4, 5.4.4 and 5.4.4.

One motivation for deriving the Wilsonian algebra is that it determines the possible topologies of the Wilson bands along \( \bar{X}\bar{U} \). This determination is through ‘rules of the curves’ that we summarize in two tables: Tab. 5.2 is derived from the algebra of \( G_{\pi,kz} \) and applies to any \( k_q \) along \( \bar{X}\bar{U} \); Tab. 5.3 is derived from \( G_X \) and applies only to \( \bar{X} \) and \( \bar{U} \).

**Wilsonian glide-reflection symmetry**

Consider the glide reflection \( \bar{M}_x \), which transforms spatial coordinates as \((x, y, z) \rightarrow (-x, y, z + 1/2)\). In App. 5.4.2, we have described how \( \bar{M}_x \) constrains Wilson loops in the \( k_x = 0 \) plane, where \( \bar{M}_x \) belongs in the little group of each wavevector, and therefore the projections on this plane separates into two mirror representations. This is no longer true for the \( k_x = \pi \) plane, since \( \bar{M}_x \) maps between two momenta which are separated by half a reciprocal period, i.e., \( \bar{M}_x : (k_y, \pi, k_z) \rightarrow (k_y, -\pi, k_z) = (k_y + \pi, \pi, k_z) - \bar{b}_2 \), as illustrated in Fig. 4.7(b). We find that the Wilson-loop operator is symmetric under a combination of a glide reflection with parallel transport over half a reciprocal period.

**Proof** By particularizing Eq. (1.26), we obtain the symmetry constraint on the projections:

\[ V(\bar{b}_2)^{-1} U_{\bar{M}_x} P(k_y, \pi, k_z) U_{\bar{M}_x}^{-1} V(\bar{b}_2) = P(k_y + \pi, \pi, k_z). \]  

(5.53)
Presently, it becomes useful to distinguish the base point of a Wilson loop, and also to define Wilson lines which do not close into a loop. The remaining discussion in this Section occurs at fixed $k_q = (\pi, k_z)$ (whose labels we suppress) and variable $k_y$. We denote the base point ($\bar{k}_y$) of a Wilson loop by the subscript in $W_{\bar{k}_y}$, and denote a Wilson line between two distinct momenta by

$$[W_{k_2 \leftarrow k_1}]_{mn} = \langle u_{m,k_2} | \prod_{k_y}^{k_2 \leftarrow k_1} P(k_y) | u_{n,k_1} \rangle. \quad (5.54)$$

Since parallel transport is unitary within the occupied subspace, [51]

$$W_{k_2 \leftarrow k_1}^\dagger W_{k_1 \leftarrow k_2} = W_{k_2 \leftarrow k_1} W_{k_1 \leftarrow k_2} = I. \quad (5.55)$$

Eq. (5.33) implies that under $\bar{M}_x$, the Wilson loop is translated by half a reciprocal period in $\vec{y}$:

$$\check{M}_x(0, -\pi) W_{-x} \check{M}_x(0, -\pi)^{-1} = W_0 \quad (5.56)$$

with

$$[\check{M}_x(0, -\pi)]_{mn} = e^{-i k_z/2} \langle u_{m,0} | V(-\check{b}_2) U_{\check{M}_x} | u_{n,-\pi} \rangle, \quad (5.57)$$

and $|u_{m,k_y,k_z}\rangle \equiv |u_{m,k_y}\rangle$. Then

$$[W_0]_{mn}$$

$$= \langle u_{m,0} | V(2\pi \vec{y}) \prod_{k_y}^{2\pi \leftarrow 0} P(k_y) | u_{n,0} \rangle = \langle u_{m,0} | \prod_{k_y}^{2\pi \leftarrow -\pi} P(k_y - 2\pi) V(2\pi \vec{y}) \prod_{k_y}^{\pi \leftarrow 0} P(k_y) | u_{n,0} \rangle$$

$$= \langle u_{m,0} | \prod_{k_y}^{0 \leftarrow -\pi} P(k_y) V(2\pi \vec{y}) \prod_{k_y}^{\pi \leftarrow -\pi} P(k_y) \prod_{k_y}^{-\pi \leftarrow 0} P(k_y) | u_{n,0} \rangle = [W_{0 \leftarrow -\pi} W_{-x} W_{-x \leftarrow 0}]_{mn}. \quad (5.58)$$

The second equality follows from Eq. (1.9) and the third from Eq. (5.55). Combining Eq. (5.56) and (5.58),

$$[\check{M}_x, W_{-x}] = 0, \quad \text{with} \quad \check{M}_x = W_{-\pi \leftarrow 0} \check{M}_x(0, -\pi). \quad (5.59)$$
To interpret this result, the Wilson-loop operator commutes with a combination of glide reflection (encoded in $\tilde{M}_x$) with parallel transport over half a reciprocal period (encoded in $W_{-\pi/2}$); we call any such ‘symmetry’ that combines a space-time transformation with parallel transport a Wilsonian symmetry, or just a W-symmetry.

Eq. (5.59) implies we can simultaneously diagonalize both Wilson-loop and W-symmetry operators; for each simultaneous eigenstate, the two eigenvalues are related in the following manner: if $\exp[i\theta]$ is the Wilson-loop eigenvalue, then the W-symmetry eigenvalue falls into either branch of $\pm i \exp[-i (k_z + \theta)/2]$, as we now prove.

**Proof** Up to a $k_z$-dependent phase factor, this W-symmetry operator squares to the reverse-oriented Wilson loop:

\[
\begin{align*}
[\tilde{M}_x^2]_{mn} &= e^{-ik_z}\langle u_m, -\pi | \prod_{k_y} P(k_y) \prod_{q_y} P(q_y + \pi) V(\tilde{b}_2)^{-1} U_{\tilde{M}_x} V(\tilde{b}_2)^{-1} U_{\tilde{M}_x} | u_n, -\pi \rangle \\
&= e^{-ik_z}\langle u_m, -\pi | \prod_{k_y} P(k_y) V(\tilde{b}_2)^{-1} V(\tilde{b}_2 - 2\pi \vec{y}) (U_{\tilde{M}_x})^2 | u_n, -\pi \rangle \\
&= -e^{-ik_z}\langle u_m, -\pi | \prod_{k_y} P(k_y) V(-2\pi \vec{y}) | u_n, -\pi \rangle = -e^{-ik_z} [W_{-\pi}]_{mn}.
\end{align*}
\] (5.60)

Here, $U_{\tilde{M}_x}^2 = -I$ represents a 2$\pi$ rotation, and in the second equality, we made use of

\[
U_{\tilde{M}_x} V(-\tilde{b}_2) = \exp[i D_{\tilde{M}_x} \tilde{b}_2 \cdot \vec{z}/2] V(-D_{\tilde{M}_x} \tilde{b}_2) U_{\tilde{M}_x} = V(\tilde{b}_2 - 2\pi \vec{y}) U_{\tilde{M}_x},
\] (5.61)

which follows from Eq. (1.29).

The situation is analogous to that of the 010-surface bands, where there are also two branches for the glide-mirror eigenvalues, namely $\pm i \exp(-ik_z/2)$. A curious difference is that the W-symmetry eigenvalue ($\lambda$) of a Wilson band also depends on the energy ($\theta$) through $\lambda = \pm i \exp[-i (k_z + \theta)/2]$.  


Wilsonian $T\bar{M}_z$-symmetry

$T\bar{M}_z$ transforms space-time coordinates as $(x, y, z, t) \rightarrow (x, y, -z + 1/2, -t)$, and momentum coordinates as $(k_y, \pi, k_z) \rightarrow (-k_y, -\pi, k_z) = (\pi - k_y, \pi, k_z) - \tilde{b}_2$, as illustrated in Fig. 4.7(d).

From Eq. (1.33) and (1.34), we obtain its action on Bloch waves:

$$\hat{T}_{\bar{M}_z}(k) = e^{-ikz/2} U_{T\bar{M}_z} K,$$  \hspace{1cm} (5.62)

and the constraint on the occupied-band projections:

$$V(\tilde{b}_2)^{-1} \hat{T}_{\bar{M}_z} P(k_y, \pi, k_z) \hat{T}_{\bar{M}_z}^{-1} V(\tilde{b}_2) = P(\pi - k_y, \pi, k_z).$$  \hspace{1cm} (5.63)

Henceforth suppressing the $k_y$ labels, we are led to

$$\hat{T}_{\bar{M}_z}(2\pi, -\pi) \mathcal{W}_{\pi < -\pi} \hat{T}_{\bar{M}_z}(2\pi, -\pi)^{-1} = \mathcal{W}_{\pi < 2\pi}$$  \hspace{1cm} (5.64)

where

$$[\hat{T}_{\bar{M}_z}(2\pi, -\pi)]_{mn} \equiv \langle u_{m,2\pi} | V(\tilde{b}_2)^{-1} \hat{T}_{\bar{M}_z} | u_{n,-\pi} \rangle,$$  \hspace{1cm} (5.65)

and $\mathcal{W}_{\pi < 2\pi}$ denotes the reverse-oriented Wilson loop with base point $2\pi$. We will use the following two identities: (i)

$$\mathcal{W}_{\pi < 2\pi} = \mathcal{W}_{2\pi < \pi} \mathcal{W}_{\pi < \pi} \mathcal{W}_{\pi < 2\pi}$$  \hspace{1cm} (5.66)

follows from a generalization of Eq. (5.58), and (ii)

$$[\mathcal{W}_{\pi < 2\pi} \hat{T}_{\bar{M}_z}(2\pi, -\pi)]_{mn}$$

$$= \langle u_{m,\pi} \prod_{k_y} P(k_y) V(\tilde{b}_2)^{-1} \hat{T}_{\bar{M}_z} | u_{n,-\pi} \rangle = \langle u_{m,-\pi} \prod_{k_y} P(k_y) V(2\pi y - \tilde{b}_2) \hat{T}_{\bar{M}_z} | u_{n,-\pi} \rangle$$

$$= \sum_{a=1}^{n_{occ}} \langle u_{m,-\pi} \prod_{k_y} P(k_y) | u_{a,0} \rangle \langle u_{a,0} | V(2\pi y - \tilde{b}_2) \hat{T}_{\bar{M}_z} | u_{n,-\pi} \rangle$$

$$\equiv \sum_{a=1}^{n_{occ}} [\mathcal{W}_{\pi < 0}]_{ma} [\hat{T}_{\bar{M}_z}(0, -\pi)]_{an}.$$  \hspace{1cm} (5.67)

Inserting (i) and (ii) into Eq. (5.64), we arrive at

$$\mathcal{T}_{\bar{M}_z} \mathcal{W}_{\pi < -\pi} \mathcal{T}_{\bar{M}_z}^{-1} = \mathcal{W}_{\pi < -\pi}, \quad \text{with} \quad \mathcal{T}_{\bar{M}_z} = \mathcal{W}_{\pi < 0} \hat{T}_{\bar{M}_z}(0, -\pi).$$  \hspace{1cm} (5.68)
The Wilson-loop operator is thus W-symmetric under $T_{\tilde{M}_z}$, which combines a space-time transformation (encoded in $\tilde{T}_{\tilde{M}_z}$) with parallel transport over half a reciprocal period (encoded in $W_{\pi \vec{e}_0}$). This constraint does not produce any degeneracy, since (i) $T^2_{\tilde{M}_z} = +I$ and furthermore (ii) the eigenvalues of $\tilde{\mathcal{M}}_x$ are preserved under $T_{\tilde{M}_z}$. To prove (i), we apply $(\tilde{T}_{\tilde{M}_z})^2 = U_{T\tilde{M}_z} U^*_{T\tilde{M}_z} = I$ to obtain

$$[T^2_{\tilde{M}_z}]_{mn} = \langle u_{m,-\pi} | \prod_{k_y} P(k_y) V(2\pi \vec{y} - \vec{b}_2) \tilde{T}_{\tilde{M}_z} \prod_{q_y} P(q_y) V(2\pi \vec{y} - \vec{b}_2) \tilde{T}_{\tilde{M}_z} | u_{n,-\pi} \rangle = \langle u_{m,-\pi} | \prod_{k_y} P(k_y) \prod_{q_y} P(q_y) | u_{n,-\pi} \rangle = W_{\pi \vec{e}_0} W_{0 \vec{e}_0} \big|_{mn} = \delta_{mn}. \quad (5.69)$$

To prove (ii), we use that $U_{\tilde{M}_z}$ and $U_{T\tilde{M}_z} K$ anticommute in the half-integer-spin representation, and therefore

$$[\tilde{\mathcal{M}}_x, T_{\tilde{M}_z}]_{mn} = e^{-ik_z} \langle u_{m,-\pi} | \prod_{k_y} P(k_y) V(-\vec{b}_2) U_{\tilde{M}_z} \prod_{q_y} P(q_y) V(2\pi \vec{y} - \vec{b}_2) u_{T\tilde{M}_z} K | u_{n,-\pi} \rangle = -e^{-ik_z} [T_{\tilde{M}_z}, W \tilde{\mathcal{M}}_x]_{mn} = e^{-ik_z} [T_{\tilde{M}_z} \tilde{\mathcal{M}}_x W]_{mn}. \quad (5.70)$$

Then define simultaneous eigenstates of $W$ and $\tilde{\mathcal{M}}_x$ such that

$$W | e^{i\theta}, \lambda; k_z \rangle = e^{i\theta} | e^{i\theta}, \lambda; k_z \rangle \quad \text{and} \quad \tilde{\mathcal{M}}_x | e^{i\theta}, \lambda; k_z \rangle = \lambda | e^{i\theta}, \lambda; k_z \rangle. \quad (5.71)$$

Once again, all operators and eigenvalues here depend on $k_z$. Finally,

$$\tilde{\mathcal{M}}_x T_{\tilde{M}_z} | e^{i\theta}, \lambda; k_z \rangle = -e^{-ik_z} T_{\tilde{M}_z} \tilde{\mathcal{M}}_x W | e^{i\theta}, \lambda; k_z \rangle = -e^{-ik_z} \lambda^* T_{\tilde{M}_z} | e^{i\theta}, \lambda; k_z \rangle = \lambda T_{\tilde{M}_z} | e^{i\theta}, \lambda; k_z \rangle. \quad (5.72)$$

In the last equality, we applied $\lambda^2 = -\exp[-i(\theta + k_z)]$. 

Effect of space-time inversion symmetry

The first two relations of Eq. (5.52) may be carried over from App. 5.4.3, if we identify $\mathcal{T}_x \equiv \hat{T}_x$. What remains is to show: $\bar{M}_x T_I = t(c\vec{z}) U_{\tilde{x}_x} \hat{T}_x |u_{n,-\pi}\rangle$.

Recalling our definitions in Eq. (5.71), we now show that $|e^{i\theta},\lambda; k_z\rangle$ and $T_I |e^{i\theta},\lambda; k_z\rangle$ belong in opposite mirror branches. To be precise, since $\lambda = \pm \exp[-i(k_z + \theta)/2]$ is energy-dependent, and $T_I$ maps $\theta \to -\theta$, we would show that $\lambda(\theta) \to -\lambda(-\theta)$:

$$\bar{M}_x T_I |e^{i\theta},\lambda; k_z\rangle = e^{-ik_z} \lambda^* T_I |e^{i\theta},\lambda; k_z\rangle = \mp ie^{-i(k_z-\theta)/2} T_I |e^{i\theta},\lambda; k_z\rangle.$$  (5.74)

Wilsonian time-reversal operator

In the remaining discussion, we particularize to two Wilson loops at fixed $k_q = (\pi,\tilde{k}_z)$, with $\tilde{k}_z = 0$ or $\pi$. Under time reversal, $(k_y,\pi,\tilde{k}_z) \rightarrow (-k_y,-\pi,-\tilde{k}_z) = (\pi-k_y,\pi,\tilde{k}_z) - \tilde{b}_2 - 2\tilde{k}_z\vec{z}$, as illustrated in Fig. 4.7(d). This implies that the occupied-band projections along these lines are constrained as

$$V(\tilde{b}_2 + 2\tilde{k}_z\vec{z})^{-1} \hat{T} P(k_y,\pi,\tilde{k}_z) \hat{T}^{-1} V(\tilde{b}_2 + 2\tilde{k}_z\vec{z}) = P(\pi-k_y,\pi,\tilde{k}_z),$$  (5.75)

where $\hat{T} = U_T K$ is the antiunitary representation of time reversal. Henceforth suppressing the $k_q$ labels, we are led to

$$\hat{T}(2\pi,-\pi) \mathcal{W}_{-x} \hat{T}(2\pi,-\pi)^{-1} = \mathcal{W}_{r,2\pi}$$  (5.76)

where

$$[\hat{T}(2\pi,-\pi)]_{mn} = \langle u_{m,2\pi} | V(\tilde{b}_2 + 2\tilde{k}_z\vec{z})^{-1} \hat{T} | u_{n,-\pi} \rangle.$$  (5.77)
and \( W_{r,2\pi} \) denotes the reverse-oriented Wilson loop with base point \( 2\pi \). Combining this result with Eq. (5.66) and the identity
\[
[W_{\pi+2\pi} \hat{T}(2\pi,-\pi)]_{mn} = \sum_{a=1}^{n_{occ}} \langle u_{m,-\pi} | -\pi \leftrightarrow 0 \prod_{k_y} \langle u_{a,0} | P(k_y) | u_{a,0} \rangle \langle u_{a,0} | V(2\pi\vec{y} - \vec{b}_2 - 2\vec{k}_z \vec{z}) \hat{T} | u_{n,-\pi} \rangle
\]
\[
\equiv \sum_{a=1}^{n_{occ}} [W_{-\pi+0}]_{ma} [\hat{T}(0,-\pi)]_{an},
\]
as follows from nearly the same manipulations in Eq. (5.67), we arrive at
\[
\mathcal{T} W_{-\pi} \mathcal{T}^{-1} = W_{-\pi}, \quad \text{with} \quad \mathcal{T} = W_{-\pi+0} \hat{T}(0,-\pi).
\]
The Wilson-loop operator is thus \( W \)-symmetric under \( \mathcal{T} \), which combines time reversal (encoded in \( \hat{T} \)) with parallel transport over half a reciprocal period (encoded in \( W_{-\pi+0} \)). A Kramers degeneracy in the spectrum follows from \( \mathcal{T}^2 = -I \):
\[
[T^2]_{mn} = \langle u_{m,-\pi} | -\pi \leftrightarrow 0 \prod_{k_y} P(k_y) \prod_{q_y} P(q_y) V(2\pi\vec{y} - \vec{b}_2 - 2\vec{k}_z \vec{z}) V(-2\pi\vec{y} + \vec{b}_2 + 2\vec{k}_z \vec{z}) (\hat{T})^2 | u_{n,-\pi} \rangle
\]
\[
= -\langle u_{m,-\pi} | -\pi \leftrightarrow 0 \prod_{k_y} P(k_y) \prod_{q_y} P(q_y) | u_{n,-\pi} \rangle = -[W_{-\pi+0} W_{0+\pi}]_{mn} = -\delta_{mn},
\]
where \( \hat{T}^2 = -I \) represents a \( 2\pi \) rotation. We further investigate if Kramers partners share identical or opposite eigenvalues under \( \tilde{M}_x \). We find at \( k_z = 0 \) that \( \mathcal{T} : \lambda \rightarrow -\lambda \), while at \( k_z = \pi \), \( \mathcal{T} : \lambda \rightarrow \lambda \). An analog of this result occurs for the surface bands, where the eigenvalues of \( \tilde{M}_x \) are imaginary (real) at \( k_z = 0 \) (resp. \( \pi \)), and time-reversal pairs up complex-conjugate eigenvalues.
Proof Applying $[\hat{T}, U_{\mathcal{M}_x}] = 0$,

$$[\mathcal{M}_x \mathcal{T}]_{mn} = e^{-ik_z/2} \langle u_{m,-\pi} | \prod_{k_y} P(k_y) V(-\vec{b}_2) U_{\mathcal{M}_x} \prod_{q_y} P(q_y) V(2\pi \vec{y} - \vec{b}_2 - 2\vec{k}_z \vec{z}) \hat{T} | u_{n,-\pi} \rangle$$

$$= e^{-ik_z/2} \langle u_{m,-\pi} | \prod_{k_y} P(k_y) \prod_{q_y} P(q_y) V(-\vec{b}_2) e^{i\vec{k}_z \cdot \vec{z}} V(2\pi \vec{y} - \vec{b}_2 - 2\vec{k}_z \vec{z}) \hat{T} U_{\mathcal{M}_x} | u_{n,-\pi} \rangle$$

$$= [\mathcal{T} \mathcal{W} \mathcal{M}_x]_{mn} = [\mathcal{T} \mathcal{M}_x \mathcal{W}]_{mn}. \quad (5.81)$$

Recalling Eq. (5.71),

$$\mathcal{M}_x \mathcal{T} |e^{i\theta}, \lambda; \vec{k}_z\rangle = \mathcal{T} \mathcal{M}_x \mathcal{W} |e^{i\theta}, \lambda; \vec{k}_z\rangle = e^{-i\theta} \lambda^* \mathcal{T} |e^{i\theta}, \lambda; \vec{k}_z\rangle = -e^{ik_z} \lambda \mathcal{T} |e^{i\theta}, \lambda; \vec{k}_z\rangle.$$

In the last equality, we applied $\lambda^2 = -\exp[-i(\theta + k_z)].$

5.5 Connectivity of bands in spin systems with glide and time-reversal symmetries

Figure 5.7: Bulk bandstructure of a spin system with glide and time-reversal symmetries. (a) either has no spin-orbit coupling, or has spin-orbit coupling with an additional spatial-inversion symmetry. (b) has spin-orbit coupling, and no spatial-inversion symmetry.

In spin systems with minimally time-reversal ($T$) and glide-reflection ($\mathcal{M}_x$) symmetries, our goal is to prove that bands divide into quadruplet sets of hourglasses, along the momentum circle parametrized by $(0, 0, k_z)$. Each quadruplet is connected, in the sense that there are enough contact points to continuously travel through all four branches. With the addition of other spatial symmetries in our space group, we further describe how degeneracies within each hourglass may be further enhanced. Our proof of connectivity generalizes
a previous proof [21] for integer-spin representations of non-symmorphic space groups.

The outline of our proof: we first consider a spin system with vanishing spin-orbit coupling, such that it has a spin $SU(2)$ symmetry. In this limit, we prove that bands divide into doubly-degenerate quadruplets with a four-fold intersection at $(0, 0, \pi)$, as illustrated in Fig. 5.7(a). Then by introducing spin-orbit coupling and assuming no other spatial symmetries, we show that each quadruplet splits into a connected hourglass (Fig. 5.7(b)).

With vanishing spin-orbit coupling, the system is additionally symmetric under the spin flip ($F_x$) that rotates spin by $\pi$ about $\vec{x}$. The double group ($G$) relations include

$$T^2 = F_x^2 = \bar{E}, \quad \bar{M}_x^2 = \bar{E} t(c\vec{z}), \quad [T, F_x] = [T, \bar{M}_x] = [F_x, \bar{M}_x] = 0,$$  \hspace{1cm} (5.82)

with $\bar{E}$ a $2\pi$ rotation and $t$ a lattice translation. It follows from this relations that we can define two operators that act like time reversal and glide reflection in a spinless system:

$$T_x \equiv T F_x, \quad \bar{m}_x \equiv \bar{M}_x F_x; \quad [T_x, \bar{m}_x] = 0, \quad T_x^2 = I, \quad \bar{m}_x^2 = t(c\vec{z}).$$  \hspace{1cm} (5.83)

These operations preserve the spin component in $\vec{z}$ – the group ($\tilde{G}$) of a single spin species (aligned in $\pm \vec{z}$) is generated by $T_x$, $\bar{m}_x$ and the lattice translations. It is known from Ref. [21] that the elementary band representation [20] of $\tilde{G}$ is two-dimensional, i.e., single-spin bands divide into sets of two which cannot be decomposed as direct sums, and in each set there are enough contact points to continuously travel through both branches; this latter property they call ‘connectivity’. We reproduce here their proof of connectivity by monodromy:

Let us consider the single-spin Bloch representation ($\tilde{D}_{k_z}$) of $\tilde{G}$ along the circle $(0, 0, k_z)$. For $k_z \neq \pi$, there are two irreducible representations (labelled by $\rho$) which are each one-dimensional:

$$\tilde{D}_{k_z}^\rho(t(c\vec{z})) = e^{-ik_z}, \quad \tilde{D}_{k_z}^\rho(\bar{m}_x) = e^{-i(k_z+2\pi\rho)/2}, \quad k_z \neq \pi, \quad \rho \in \{0, 1\},$$  \hspace{1cm} (5.84)
as follows from Eq. (5.83). Making one full turn in this momentum circle \((k_z \rightarrow k_z + 2\pi)\) effectively permutes the representations as \(\rho \rightarrow \rho + 1\). This implies that if we follow continuously an energy function of one of the two branches, we would evolve to the next branch after making one circle, and finally return to the starting point after making two circles – both branches form a connected graph. The contact point between the two branches is determined by the time-reversal symmetry \((T_x)\), which pinches together complex-conjugate representations of \(\bar{m}_x\) at \(k_z = \pi\); on the other hand, real representations at \(k_z = 0\) are not degenerate. We applied here that \([T_x, \bar{m}_x] = 0\), and the eigenvalues of \(\bar{m}_x\) are imaginary (real) at \(k_z = \pi\) (resp. 0).

Due to the spin \(SU(2)\) symmetry, we double all irreducible representations of \(\hat{G}\) to obtain representations of \(G\), i.e., in the absence of spin-orbit coupling but accounting for both spin species, bands are everywhere spin-degenerate, and especially four-fold degenerate at \(k_z = \pi\). Recall that the eigenvalues of \(\bar{M}_x\) fall into two branches labelled by \(\eta = \pm 1\) in \(\lambda_x(k_z) = \eta i \exp(-ik_z/2)\). For each spin-degenerate doublet, the two spin species fall into opposite branches of \(\bar{M}_x\), as distinguished by solid and dashed curves in Fig. 5.7(a). This result follows from continuity to \(k_z = 0\), where Kramers partners have opposite, imaginary eigenvalues under \(\bar{M}_x\).

Without additional spatial symmetries, the effect of spin-orbit coupling is to split the spin degeneracy for generic \(k_z\), while preserving the Kramers degeneracy at \(k_z = 0\) and \(\pi\) – the final result is the hourglass illustrated in Fig. 5.7(b). To demonstrate this, we note at \(k_z = \pi\) that each four-dimensional subspace (without the coupling) splits into two Kramers subspace, where Kramers partners have identical, real eigenvalues under \(\bar{M}_x\). Pictorially, two solid curves emerge from the one of the two Kramers subspaces, and for the other subspace both curves are dashed. Furthermore, we know from the previous paragraph that each Kramers pair at \(k_z = 0\) combines a solid and dashed curve. These constraints may be interpreted as curve boundary conditions at 0 and \(\pi\), which impose a solid-dashed crossing.
between the boundaries. There is then an ‘unavoidable degeneracy’ [20] which can move along the half-circle, but cannot be removed. This contact point, in addition to the unmovable Kramers degeneracies at 0 and $\pi$, guarantee that each quadruplet is connected.

We end by considering how other spatial symmetries (beyond $\tilde{M}_x$) may enhance degeneracies within each hourglass. For illustration, we consider the spatial inversion ($I$) symmetry, which applies to the space group of KHgX. Since $TT$ belongs in the group of every bulk wavevector, the spin degeneracy along $(0,0,k_z)$ does not split, and $k_z = \pi$ remains a point of four-fold degeneracy.

### 5.6 Introduction to group extensions by Wilson loops

In Sec. 5.3, we introduced three groups:

(i) $G_s$ is a symmorphic, spinless group generated by time reversal ($T$), a glideless reflection ($M_x$) and spatial inversion ($I$).

(ii) The group ($G_{\tilde{X}}$) of the Wilson loop is generated by $2\pi$-rotation ($\tilde{E}$), a lattice translation ($t(c\vec{z})$), the Wilson loop ($W$), and analogs of time reversal ($\tilde{T}$), glide reflection ($\tilde{M}_x$) and spatial inversion ($I$) that additionally encode parallel transport.

(iii) $N$ is a group generated by $\tilde{W}$, $\tilde{E}$ and $t(c\vec{z})$. Eq. (5.9) informs us that $N$ is a normal subgroup of $G_{\tilde{X}}$.

We would like to show that $G_{\tilde{X}}$ is an extension of $G_s$ by $N$. It is sufficient to show that $G_s$ is isomorphic to the factor group $G_{\tilde{X}}/N$. This factor group has as elements the left cosets $gN$ with $g \in G_{\tilde{X}}$; by the normality of $N$, $gN = Ng$. This isomorphism respectively maps the elements $N$, $TN$, $\tilde{M}_x N$ (in $G_{\tilde{X}}/N$) to $I, T, M_x$ (in $G_s$); this is a group isomorphism in the sense that their multiplication rules are identical. For example, $M_x^2 = I$ is isomorphic to:

\[
(\tilde{M}_x N)^2 = \tilde{M}_x (N \tilde{M}_x) N = \tilde{M}_x^2 N^2 = \tilde{E} t(c\vec{z}) W^{-1} N = N, \quad (5.85)
\]
where we applied that $\mathcal{N}$ is a normal subgroup of $G_{\tilde{\chi}}$. Two extensions are equivalent if there exists a group isomorphism between them; $H^2(G_s, \mathcal{N})$ classifies the isomorphism classes of all extensions of $G_s$ by $\mathcal{N}$, of which $G_{\tilde{\chi}}$ is one example.

For a simple example of $H^2(G, \mathcal{N})$, consider a reduced problem where we extend

$$G = \{I, T, M_x, TM_x\}$$

by a group of Wilson loops

$$\mathcal{N} = \{\mathcal{W}^n \mid n \in \mathbb{Z}\}.$$  (5.87)

$G$ acts on $\mathcal{N}$ as

$$T \mathcal{W} T^{-1} = \mathcal{W}^{-1} \quad \text{and} \quad M_x \mathcal{W} M_x^{-1} = \mathcal{W}.$$  (5.88)

The algebra of $G$ (described in Eq. (5.17)) may be extended as

$$M_x^2 = \mathcal{W}^a; \quad T^2 = \mathcal{W}^b \quad \text{and} \quad M_x T = \mathcal{W}^c T M_x,$$  (5.89)

with $a, b, c$ integers that we proceed to constrain. $b = 0$ follows from associativity of $T^3$:

$$T \mathcal{W}^b = T(TT) = (TT)T = \mathcal{W}^b T = T \mathcal{W}^{-b}.$$  (5.90)

$a = c$ follows from

$$\mathcal{W}^a T = M_x^2 T = \mathcal{W}^{2c} T M_x^2 = \mathcal{W}^{2c} T \mathcal{W}^a = \mathcal{W}^{2c-a} T.$$  (5.91)

Moreover, only the parity of $a$ is invariant, since by a gauge transformation,

$$M_x^2 = \mathcal{W}^a \rightarrow (M_x \mathcal{W}^{n(M_x)})^2 = \mathcal{W}^a \quad \text{with} \quad n(M_x) \in \mathbb{Z}.$$  (5.92)

The two elements of $H_2(G, \mathcal{N})$ are then distinguished by $a = 0$:

$$M_x^2 = I, \quad T^2 = I, \quad [T, M_x] = 0.$$  (5.93)
and $a = -1$:

$$M_x^2 = W^{-1}, \quad T^2 = I, \quad T M_x = W^{-1} M_x T.$$  \hfill (5.94)

Note that we have rederived Eq. (5.12) and (5.15), modulo factors of $\bar{E}$ and $t(c\vec{z})$. The first extension is split (i.e., it is isomorphic to a direct product of $G$ with $N$), and corresponds to the identity element of $H_2(G, N) \cong \mathbb{Z}_2$. Multiplication of two elements corresponds to multiplying the factor systems, e.g., the two non-split elements multiply as

$$M_x^2 = W^{-2}, \quad T^2 = I, \quad T M_x = W^{-2} M_x T,$$  \hfill (5.95)

which is gauge-equivalent to Eq. (5.93).

5.7 Discussion and outlook

Our theory introduces the notion of piecewise topological insulators, where sub-topologies on different high-symmetry submanifolds of the Brillouin zone must be pieced together to form a global topology. We propose a general methodology to classify piecewise topologies using the Wilson loop – our proposed program amounts pictorially to interpolating and matching curves.

Our non-symmorphic theory presents the first case study where group cohomology is applied to the theory of band insulators. However, the non-symmorphicity is not a prerequisite for its application, e.g., there are glide-less mirror planes (in face-centered cubic lattices) where the symmetry also relates momentum-separated Bloch waves; the implications, if any, are left to future study. Our application of group cohomology may be compared with the classification of 1D symmetry-protected, bosonic systems [77] – there, (i) groups are extended by a $U(1)$ subgroup which reflects a gauge ambiguity in quantum wavefunctions, (ii) projective representations only describe boundaries of the 1D system, and (iii) the ordinary (projective) representation is in one-to-one correspondence with a trivial (resp. topological) phase. In our band-theoretical context, (i) the crystal group is extended by a subgroup
of Wilson loops, (ii) projective representations only describe the bulk of the crystal, and (iii) the different representations (ordinary and projective) correspond to different sets of available topologies; the exact topology is specified by details of the Hamiltonian.
Chapter 6

Wilson-Loop Characterization of
Inversion-Symmetric Topological
Insulators

In the last two chapters, we dealt with insulators with discretely robust surface properties. However, a more sensitive probe of topology is through bulk Wilson loops – some topological phases have quantized transport properties (specifically, quantization of Wilson-loop eigenvalues), but no interesting surface properties. Quantization is made possible by the simplest spatial symmetry: inversion.

To motivate the physical significance from a related perspective, we remind the reader that a topological insulator cannot be continuously transformed to a direct-product state. This corresponds to a limit where all hoppings between atoms are turned off, so the ground state is a direct product of atomic wavefunctions. Such a limit is easily stated for a monatomic Bravais lattice: all band eigenfunctions are independent of crystal momentum, and parallel transport is trivial, i.e., the Wilson loop $W$ equals the identity in the occupied subspace. Then a sufficient criterion for nontriviality is that a subset of the $W$-eigenspectrum is robustly fixed to a value other than $+1$. In this chapter we demonstrate that some 1D $I$-symmetric insulators have a number ($\mathcal{R}$) of $W$-eigenvalues that are symmetry-
fixed to $-1$. This number $\mathcal{R} \in \mathbb{Z}^\geq$ classifies the 1D insulator; here, $\mathbb{Z}^\geq$ denotes the set of nonnegative integers. $\mathcal{R}$ is completely determined by the symmetry representations of the occupied wavefunctions at inversion-invariant momenta – momenta which satisfy $k = -k$ up to a reciprocal lattice vector. The even-parity (odd-parity) wavefunctions are defined to have inversion eigenvalues $+1$ ($-1$). If there are $n_{(-)}(0)$ odd-parity wavefunctions at momentum $k = 0$ and $n_{(-)}(\pi)$ of them at $k = \pi$, we find that $\mathcal{R}$ quantifies a change in the group representations between 0 and $\pi$:

$$\mathcal{R} = |n_{(-)}(0) - n_{(-)}(\pi)|. \quad (6.1)$$

In 1D, the inversion eigenvalues tell the whole story. Is this also true for the 2D insulator? No, we find there exists insulators with the same inversion eigenvalues, but with distinct band structures. A case in point is an $\mathcal{I}$-symmetric insulator with Chern number 2 – it is a time-reversal breaking insulator which displays a quantum anomalous Hall effect. [2] In the geometric-phase theory of polarization, the non-Abelian Berry phases are identified as centers of charge, and they are functionally dependent on an adiabatic parameter. [47] For a Chern insulator, these phases are known to have a center-of-mass winding number, as plotted in Fig. 6.1-a; this implies a net transfer of charge in one adiabatic cycle. In Fig. 6.1-b, the Berry phases are strikingly different, yet they correspond to an insulator with the same inversion eigenvalues. The Berry phases come in pairs, and each member of a pair winds in a direction opposite to the other member. We identify this insulator as having a nontrivial relative winding number $W$, which is protected only by inversion symmetry; $W$ provides a $\mathbb{Z}^\geq$ classification of the 2D insulator. Both insulators of Fig. 6.1-a and -b share in common that their Berry phases interpolate across the maximal possible range $[0, 2\pi)$ in one adiabatic cycle. Such a property, called spectral flow, is shared by all Chern insulators, and also the time-reversal invariant $\mathbb{Z}_2$ insulators. [8, 71, 78] In this sense, $W$ is the inversion-analog of the first Chern class and the $\mathbb{Z}_2$ invariant.

Our findings are relevant to the theory of maximally-localized Wannier functions (MLWF). In 1D, Berry phases represent spatial coordinates of the MLWF. In higher dimensions, these phases are the spatial coordinates of hybrid WF’s, which maximally localize along one di-
Figure 6.1: Non-Abelian Berry phases for four distinct insulators. Each figure contains three unit cells in an effective 1D-lattice along $\hat{x}$; we track the real-space trajectories of the phases (blue circles) in $\hat{x}$ as momentum $k_y$ is varied through two adiabatic cycles. (a) An insulator with Chern number $C_1 = 2$ and zero relative winding ($W$); this is modeled by the Hamiltonian (6.7) with parameters $m = 3$ and $\delta = 2$. (b) An insulator with relative winding $W = 1$ and zero $C_1$; this is modeled by Eq. (6.7) with $m = 3$ and $\delta = 1$. (c) $W = 2$ and $C_1 = 0$; this is modeled by Eq. (6.11). (d) $W = 0$ and $C_1 = 0$; the insulator has a nontrivial polarization, and is modeled by Eq. (6.4) with parameters $\alpha = -1.5, \beta = 1.5, \delta = -1$.

rection, but extend in the remaining directions as a Bloch wave. [30, 31] The applications of MLWF’s and their hybrid cousins are manifold: to name a few examples, they are used to analyze chemical bonding, and to locally probe electric polarization and orbital magnetization. [79] In our chapter, we derive a mapping between inversion eigenvalues and Berry phases, which strongly constrains the (hybrid) MLWF’s of any inversion-symmetric insulator. Our result is an extension of Kohn’s single-band result to insulators with interband degeneracies, such as those enforced by time-reversal symmetry. [80,81]

While we explicitly discuss insulators, our results may be generalized to any system, fermionic or bosonic, with discrete translational symmetry and an energy gap. Examples include photonic crystals with a bandgap, and cold atoms in an optical lattice. The dimension in ‘1D (2D) insulator’ refers to that in momentum space. Thus, ‘1D (2D) insulator’
may refer to a material of larger spatial dimension, but with a 1D (2D) Brillouin zone; in such cases ‘inversion symmetry’ in 1D (2D) must be understood as a mirror ($C_2$ rotational) symmetry. A case in point is a 3D optical lattice which is periodic only in $\hat{x}$, and is symmetric under $x \to -x$. Moreover, our results also apply to 1D and 2D submanifolds embedded in larger-dimensional Brillouin zones. These are submanifolds which are mapped to themselves under mirror or $C_2$ rotation. For example, a plane of constant $k_z = 0$ in a 3D $I$-symmetric insulator may possess a nontrivial relative winding.

The outline of the next few Sections: we analyze the 1D $I$-symmetric insulator in Sec. 6.1. Here, we (i) derive a mapping between $I$ and $W$ eigenvalues, (ii) formulate the topological index $R \in \mathbb{Z}_{\geq}$, and establish a connection between $R$ and the entanglement spectrum. We analyze the 2D $I$-symmetric insulator in Sec. 6.2. Here, we (a) analyze Chern insulators and $Z_2$ insulators with inversion symmetry, (b) and identify a relative winding number $W \in \mathbb{Z}_{\geq}$ which characterizes $I$-protected spectral flow. Sec. 6.3 to 6.7 provides supplemental derivations as well as models. We conclude in Sec. 6.8 with a discussion of the experimental implications.

6.1 Wilson-loop characterization of the 1D Inversion-symmetric insulator

We highlight distinctive features of the $I$-symmetric Wilson loop (Sec. 6.1.1), and present a mapping between the $W$-eigenvalues and the $I$ eigenvalues of the ground state (Sec. 6.1.2). In Sec. 6.1.3, we formulate the topological index $R \in \mathbb{Z}_{\geq}$ that classifies $I$-symmetric insulators. In addition, we relate $R$ to a well-known $Z_2$ index that distinguishes the electric responses of these insulators.

6.1.1 Constraints on the Wilson Loop due to Inversion Symmetry

In 1D, inversion maps the spatial coordinate $x \to -x$; we choose the center of inversion as the spatial origin ($x = 0$). We define the unit cell such that the unit cell enclosing the
spatial origin is mapped to itself under inversion. At inversion-invariant momenta (0 and \( \pi \)), the wavefunctions transform in irreducible representations of inversion – even-parity (odd-parity) wavefunctions are defined to have inversion eigenvalues +1 (−1). Due to the discrete translational symmetry, an inversion center at the origin implies existence of inversion centers at \( x = 1/2, 1, 3/2, 2 \ldots \), in units where the distance between two unit cells is unity. For any integer \( n \), we call \( x = n \ (x = n + 1/2) \) a primary (secondary) site.

As shown in Sec. 1.2, a tight-binding Hamiltonian with \( \mathcal{I} \) symmetry satisfies \( \varphi h(k) \varphi = h(-k) \), where \( \varphi \) is the representation of inversion in the basis of Löwdin orbitals. This symmetry implies that the set of \( \mathcal{W} \)-eigenvalues is equal to its complex conjugate. Equivalently, the eigenvalues of \( \mathcal{W} \) are constrained to \( \pm 1 \) or otherwise form complex-conjugate pairs. Such a constraint may be intuited from the theory of MLWF’s: the MLWF’s (i) are centered at the primary site (+1) or (ii) at the secondary site (-1) or (iii) form pairs that center equidistantly on opposite sides of a primary site (\( \lambda \lambda^* \)). In all three cases, the periodic configuration of Wannier centers is invariant under a spatial inversion \( x \to -x \). The derivation of this constraint is left to Sec. 6.3.

### 6.1.2 1D: Mapping between Wilson-loop and Inversion Eigenvalues

**Definition:** For the occupied bands of an insulating phase, let us define the number of even- and odd-parity wavefunctions at \( k^\text{inv} = \{0, \pi\} \), as \( n_{(+)}(k^\text{inv}) \) and \( n_{(-)}(k^\text{inv}) \) respectively. Given this set of four numbers \( \{n_{(+)}(0), n_{(-)}(0), n_{(+)}(\pi), n_{(-)}(\pi)\} \), we identify the smallest of the four and label it as \( n_s \), i.e., \( n_s \) counts the fewest bands of one parity (FBOP) among both symmetric momentum \( k^\text{inv} \). \( n_s = 0 \) if all the occupied wavefunctions at \( k = 0 \) (or \( \pi \)) have the same parity. We label the momentum where FBOP lies as \( k_s \) and the \( \mathcal{I} \) eigenvalue of FBOP as \( \xi_s \). Let us identify the FBOP for the following examples.

(a) Consider a two-band insulator with \( \mathcal{I} \) eigenvalues \((++)\) at \( k = 0 \) and \((+-)\) at \( k = \pi \). The FBOP are the negative-\( \mathcal{I} \) bands at \( k_s = 0 \). None exists, so \( n_s = 0 \).

(b) Suppose we had a four-band insulator with \( \mathcal{I} \) eigenvalues \((++--)\) at \( k = 0 \) and
(+ + +) at \( k = \pi \), the FBOP is the single negative-I band at \( k_s = \pi \), so \( \xi_s = -1 \) and \( n_s = 1 \).

(c) If a subset of the four numbers \( \{ n(\epsilon)(k^{\text{inv}}) \} \) are equally small, we may denote any number in this subset as \( n_s \). In a two-band example, we may encounter \( n_{(+)}(0) = n_{(-)}(0) = n_{(+)}(\pi) = n_{(-)}(\pi) = 1 \). Then, one may label any of the four possibilities as the FBOP.

**Mapping:** Given an inversion-symmetric insulator that is characterized by the quantities \( \{ n(\epsilon)(k^{\text{inv}}), n_s, k_s, \xi_s \} \), its Wilson-loop eigenspectrum consists of:

(i) \( (n_{(+)}(k_s + \pi) - n_s) \) number of \(-\xi_s\) eigenvalues,

(ii) \( (n_{(-)}(k_s + \pi) - n_s) \) number of \( \xi_s \) eigenvalues, and

(iii) \( n_s \) pairs of complex-conjugate eigenvalues.

In the above examples, the \( \mathcal{W} \)-spectrum of insulator (a) comprises one +1 and one -1 eigenvalue; for insulator (b), there are one +1 eigenvalue, one -1 eigenvalue, and one complex-conjugate pair; insulator (c) has one complex-conjugate pair only. The proof of this mapping is detailed in Sec. 6.5. The interested reader also may refer to Sec. 6.4, where we undertake the case studies of the one- and two-band \( \mathcal{W} \)'s; these case studies offer an intuitive understanding of the above mapping, and also provide an alternate derivation that is specific to one and two occupied bands. For an insulator with one, two and four occupied bands, we tabulate the possible mappings in Tab. 6.1, 6.2 and 6.3 respectively. We have described a mapping from \( \mathcal{I} \)- to \( \mathcal{W} \)-eigenvalues; the reverse mapping is possible up to some arbitrariness. This is because the \( \mathcal{W} \)-spectrum is sensitive only to changes in the representations between 0 and \( \pi \), and is invariant under: (i) multiplication of all \( \mathcal{I} \)-eigenvalues by a common factor -1, and (ii) interchanging the \( \mathcal{I} \)-eigenvalues at 0 with those at \( \pi \).

Let us define a \( \mathbb{Z}^\geq \) index, \( \mathcal{R} \), as the number of -1 eigenvalues in the \( \mathcal{W} \)-spectrum. It is possible that one or more pairs of complex-conjugate eigenvalues are accidentally degenerate at -1; we exclude them from the definition of \( \mathcal{R} \). Through the above mapping, we deduce
that $\mathcal{R}$ is the absolute difference in the number of same-symmetry bands between 0 and $\pi$, and quantifies the change in the group representation; cf. Eq. (6.1). In the following Section, we argue that a nonzero $\mathcal{R}$ is an indication of topological nontriviality.

<table>
<thead>
<tr>
<th>$\mathcal{I}$ eigenvalues</th>
<th>$\mathcal{W}$-spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>{$(+) (+)$}</td>
<td>[+]</td>
</tr>
<tr>
<td>{$(+) (-)$}</td>
<td>[−]</td>
</tr>
</tbody>
</table>

Table 6.1: For an insulator with one occupied band, we tabulate the $\mathcal{I}$ eigenvalues of the occupied band at symmetric momenta $\{0, \pi\}$ and the corresponding $\mathcal{W}$-spectrum. $+$ (−) refers to an eigenvalue of $+1$ ($-1$). $\{(+) (-)\}$ may refer to either (i) a positive-$\mathcal{I}$ band at $k = 0$, with a negative-$\mathcal{I}$ band at $\pi$, or (ii) a negative-$\mathcal{I}$ band at 0, with a positive-$\mathcal{I}$ band at $\pi$. If two sets of $\mathcal{I}$ eigenvalues (from two distinct insulators) are related by a global change in sign, they are mapped to the same $\mathcal{W}$ eigenvalue. For example, both $\{(+) (+)\}$ and $\{(-) (-)\}$ are mapped to $\mathcal{W} = +1$.

<table>
<thead>
<tr>
<th>$\mathcal{I}$ eigenvalues</th>
<th>$\mathcal{W}$-spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i) ${(++) (++})$</td>
<td>[++]</td>
</tr>
<tr>
<td>(ii) ${(++) (++})$</td>
<td>[−−]</td>
</tr>
<tr>
<td>(iii) ${(++) (+−)}$</td>
<td>[λλ*]</td>
</tr>
<tr>
<td>(iv) ${(+) (+−)}$</td>
<td>[λλ*]</td>
</tr>
</tbody>
</table>

Table 6.2: For an insulator with two occupied bands, we tabulate the $\mathcal{I}$ eigenvalues of the occupied bands at symmetric momenta $\{0, \pi\}$ and the corresponding $\mathcal{W}$-spectrum. We collect the $\mathcal{I}$ eigenvalues $\xi_i$ at each symmetric momenta into $(\xi_1 \xi_2)$.

6.1.3 1D: Topological Invariants from the Wilson Loop

$\mathbb{Z}$ Index: Number of Robust -1 Wilson-Loop Eigenvalues

A topological insulator cannot be continuously transformed to a direct product of atomic wavefunctions. For a monatomic Bravais lattice, the wavefunctions of a direct-product state are independent of crystal momentum. We deduce from (2.9) that $\mathcal{W}$ equals the identity, or that the MLWF’s are centered at the primary site, where the atom lies – we call this the atomic limit. A nonzero $\mathcal{R}$ index obstructs $\mathcal{W}$ from being tuned to the identity; this is a sufficient condition for nontriviality. While complex-conjugate $\mathcal{W}$-eigenvalues $[\lambda, \lambda^*]$ also deviate from the atomic value of $+1$, they are not a sufficient condition for nontriviality.
Table 6.3: For an insulator with four occupied bands, we tabulate the \( I \) eigenvalues of the occupied bands at symmetric momenta \( \{0, \pi\} \) and the corresponding \( W \)-spectrum. We collect the \( I \) eigenvalues \( \xi_i \) at each symmetric momenta into \((\xi_1 \xi_2 \xi_3 \xi_4)\).

The exact value of \( \lambda \) is not fixed by symmetry; this arbitrariness reflects the range in this equivalence class, \textit{i.e.}, it is possible to tune the Hamiltonian and sweep the interval of allowed \( \lambda \) while preserving both gap and symmetry. In particular, we can always tune the complex-conjugate eigenvalues to the trivial limit of \([+1, +1]\). It is possible that pairs of complex-conjugate eigenvalues are accidentally degenerate at -1. Unlike the \( R \) values of -1, these extra degeneracies are not protected by \( I \) – they generically destabilize under a soft deformation of the ground-state, hence they do not indicate a nontrivial phase. Hence, symmetry dictates that \( N_{(-1)} \) is the minimum number of \( -1 \) eigenvalues; there are two implications:

(i) Suppose we begin with a nontrivial insulator with \( R > 0 \), and we would like to transform it to an atomic insulator while preserving \( I \) symmetry. The energy gap must close a minimum of \( R \) times at a symmetric momentum, before the atomic limit (\( R = 0 \)) is reached. In each gap-closing event, a pair of opposite-sign \( I \)-eigenvalues are inverted between occupied and unoccupied bands, thus reducing \( R \) by one.

(ii) Let us establish a connection between holonomy and entanglement. Turner \textit{et al.} have demonstrated that 1D \( I \)-symmetric insulators manifest modes that robustly localize at boundaries created by a spatial entanglement cut. [83] As demonstrated in Ref. [73] and [74], the number \((\chi \in \mathbb{Z}^\geq)\) of stable modes at each entanglement boundary is equal
to the absolute difference in the number of same-symmetry bands between 0 and $\pi$. Thus, we identify $\chi$ with the $W$-index $R$, and show that the two formulations of nontriviality are equivalent. The presence of these mid-gap modes ensure that the entanglement entropy can never be tuned to zero by any gap- and symmetry-preserving transformation – this has been proposed as a criterion for nontriviality that unifies all known topological insulators. [63,73]

The story is not so different with multiple atoms per unit cell, which constitute a molecule. In the limit of isolated molecules, inversion symmetry within a molecule imposes that the MLWF’s are symmetric about the primary site (which is not necessarily where an atom sits). That is, each Wannier center either lies on the primary site, or form equidistant pairs on either side of it. Equivalently, the allowed $W$-eigenvalues of a direct-product state are 1 and $\{\lambda, \lambda^*\}$. If $N_{(-1)} > 0$, this indicates a Wannier center at the secondary site, which can only arise from nontrivial interactions between molecules.

$Z_2$ Polarization Index: Determinant of $W$

The determinant of $W$, which we define as $D$, is the exponentiated polarization of the 1D insulator. Since all $W$-eigenvalues are either $\pm 1$ or form complex-conjugate pairs, $D$ is quantized to $\pm 1$ - the classification of the electric response is $Z_2$, as is recognized in works such as Ref. [29, 73]. Moreover, $D$ is only determined by the number of -1 eigenvalues: $D = (-1)^{N_{(-1)}}$. Let us relate $D$ to the $\mathcal{I}$ eigenvalues of the ground state. From (6.1) we have that

$$D = (-1)^{|n_{(-0)}(\pi) - n_{(-\pi)}(0)|} = \prod_{k^{\text{inv}}=0,\pi}^{n_{\text{occ}}} \prod_{m=1}^n \xi_{k^{\text{inv}}}^m,$$

(6.2)

where $\xi_{k^{\text{inv}}}^m$ is the $\mathcal{I}$ eigenvalue of the $m$’th band at symmetric momentum $k^{\text{inv}}$. This concludes our discussion for 1D.
6.2 Wilson-loop characterization of the 2D Inversion-Symmetric Insulator

The Wilson loop $W$ is known to encode the first Chern class $C_1$; we present a summary of this relation in Sec. 6.2.1. In Sec. 6.2.2, we impose $I$ symmetry and investigate how the symmetry constrains $W$ and the allowed Chern numbers. $W$ is further constrained if the insulator is also time-reversal symmetric (TRS) – this is explored in Sec. 6.2.3. In Sec. 6.2.4, we introduce a relative winding number $W$ that characterizes insulators with $I$-protected spectral flow.

Figure 6.2: The Wannier center flows for a 2D insulator with $I$ symmetry. Each figure contains three unit cells in an effective 1D-lattice along $\hat{x}$; the positions of the primary sites are indicated by black dots. The ground state contains two occupied bands, hence there are two Wannier centers in each unit cell. (a) This phase is realized in the model Hamiltonian (6.4), with parameters $\alpha = -1.5$, $\beta = 1.5$ and $\delta = 1$. Upon $k_y \rightarrow k_y + 2\pi$, the pair of Wannier centers in each unit cell exchange positions. There is no net transfer of charge between unit cells, hence $C_1 = 0$. (b) This phase is realized in the same model with $\alpha = -1.5$ and $\beta = 0$. Upon $k_y \rightarrow k_y + 2\pi$, one Wannier center adiabatically flows to its neighboring unit cell on the left. This represents a quantized Hall current, hence $C_1 = -1$.

6.2.1 Wilson Loops and the First Chern Class

A well-known relation exists between Wilson loops and the integer quantum Hall effect. Let us apply an electric field along $\hat{y}$, which adiabatically translates all single-particle states in
the parameter space \( k_y \). To probe for a quantum Hall response, we study the \( k_y \)-evolution of the ground-state polarization (in \( \hat{x} \)) – we are interested in Brillouin-zone \( W \)'s at constant \( k_y \): \( W_{k_y} = T \exp (-\int d k_x C_x(k)) \). Let us denote the \( n_{occ} \) eigenvalues of \( W_{k_y} \) by the set \( \{ \exp (i \vartheta^m_{k_y}) \} \). The geometric phase \( \vartheta^m_{k_y}/2\pi \) represents the center of a hybrid Wannier function (WF), which extends in \( \hat{y} \) in the manner of a 1D Bloch wave, but localizes in \( \hat{x} \) as a 1D WF; we refer to these phases as the Wannier centers. [47–49, 84, 85] These hybrid WF’s are similar to classical line charges; the quantum-mechanical electron density may be represented by a lattice of line charges. The derivative of the geometric phase, \( \dot{\vartheta}^m_{k_y} \equiv d \vartheta^m/d k_y \), is interpreted as the real-space velocity (in \( \hat{x} \)) of the \( m \)'th Wannier center at time \( k_y \). By integrating the velocities of all Wannier centers over a period \( 2\pi \), we obtain the net quantum Hall current. Thus, we identify the first Chern class as the center-of-mass winding: [37, 86–91]

\[
C_1 = \sum_{m=1}^{n_{occ}} \int \dot{\vartheta}^m_{k_y} \frac{d k_y}{2\pi}.
\] (6.3)

As we have shown in Sec. 2.2, polarization is directly related to the continuum Wilson loop, which is defined in (2.9). However, the winding number in the tight-binding Wilson loop, as defined in Sec. 2.3, is identical to that in the continuum Wilson loop. This follows because their connections differ by an operator that is periodic in \( k_y \) (cf. Eq. (2.23) ). For the purpose of computing Chern numbers, both Wilson loops give identical results.

For illustration, we consider the 4-band model

\[
h(k) = \frac{1}{2} \Gamma_{13} + \frac{\alpha}{2} (\cos k_x + \cos k_y) (\Gamma_{30} + \Gamma_{03})
+ (\Gamma_{12} + \Gamma_{31}) \sin k_x + (\Gamma_{21} + \Gamma_{32}) \sin k_y - \Gamma_{03}
+ \frac{\beta}{2} (\cos k_x) (\cos k_y - \delta) (\Gamma_{03} - \Gamma_{30}),
\] (6.4)

where \( h(k) \) is a matrix in the tight-binding basis. \( \Gamma_{ij} \) are defined as \( \sigma_i \otimes \tau_j \); \( \sigma_0 \) \( (\tau_0) \) is the identity in spin (orbital) space; \( \sigma_{i=1,2,3} \) \( (\tau_{i=1,2,3}) \) are Pauli matrices in spin (orbital) space. The Hamiltonian possesses an \( I \) symmetry: \( \Gamma_{03} h(k) \Gamma_{03} = h(-k) \). The Fermi energy is chosen so that there are two occupied bands in the ground state. We tabulate the \( I \)
and $W$-eigenvalues for various choices of the parameters $(\alpha, \beta$ and $\delta)$ in Tab. 6.4. In Fig. 6.2-a we plot the $W_{k_y}$-spectrum for a trivial insulator ($\alpha = -1.5, \beta = 1.5, \delta = 1$); Fig. 6.2-b corresponds to a nontrivial insulator with $C_1 = -1$ ($\alpha = -1.5, \beta = 0, \delta = 0$).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>$I$ eigenvalues</th>
<th>$W_{K_y}$ eigenvalues</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>$\beta$</td>
<td>$\delta$</td>
</tr>
<tr>
<td>-1.5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>-1.5</td>
<td>1.5</td>
<td>1</td>
</tr>
<tr>
<td>-1.5</td>
<td>1.5</td>
<td>-1</td>
</tr>
</tbody>
</table>

Table 6.4: The $I$ and $W_{K_y}$ eigenvalues of the ground state of Hamiltonian (6.4), for various parameters.

### 6.2.2 The Inversion-Symmetric Wilson Loop and the Integer Quantum Hall Effect

Let us investigate the spectrum of the $I$-symmetric $W_{k_y}$. As derived in Sec. 6.6, we find that $W_{k_y}$ is equivalent to the Hermitian adjoint of $W_{k_y}$ by a unitary transformation, i.e., the sets of $W$-eigenvalues at $\pm k_y$ are equal up to complex conjugation:

$$\{\exp i\vartheta_{k_y}\} = \{\exp -i\vartheta_{k_y}\},$$

as may be verified in Fig. 6.2. At $K_y \in \{0, \pi\}$, the 1D line of states behaves like a 1D $I$-symmetric insulator in two respects: (i) the eigenvalues of $W_{K_y}$ are constrained to $\pm 1$ or otherwise form complex-conjugate pairs. (ii) In 1D, the $I$ eigenvalues at $k = 0$ and $\pi$ are related to $W$-eigenvalues through the mapping of Sec. 6.1.2; in 2D, the $I$ eigenvalues at momenta $(0, K_y)$ and $(\pi, K_y)$ are related to the eigenvalues of $W_{K_y}$ through the same mapping.

Let us define the number of robust $-1$ eigenvalues in the spectra of $W_0$ and $W_\pi$ as $N_{(-1)}(0)$ and $N_{(-1)}(\pi)$ respectively. During the adiabatic evolution, $R(K_y)$ is the number of Wannier centers that localize at each secondary site at time $K_y$. A difference in the indices $N_{(-1)}(0)$ and $N_{(-1)}(\pi)$ implies a net Hall current; moreover, the parity of the Chern number
is determined through

\[ \mathcal{R}(0) - \mathcal{R}(\pi) = C_1 \mod 2. \quad (6.6) \]

The two parities of \( C_1 \) correspond to the following situations:

(i) Suppose the parities of \( N_{(-1)}(K_y) \) differ. Between \( K_y = 0 \) and \( \pi \), an odd number of Wannier centers must interpolate between the secondary sites (\( \mathcal{W} \)-eigenvalue of \(-1\)) and the non-secondary sites, which include (a) the primary sites (+1) (see Fig. 6.2-b), and (b) the complex-conjugate sites (\( \lambda \lambda^* \)). The net translation of Wannier centers in the interval \( k_y \in [0, \pi] \) is half an odd integer. It follows from (6.3) and (6.5) that \( C_1 \) is odd.

(ii) An analogous argument emerges when the parities of \( N_{(-1)}(K_y) \) are equal. Now an even number of Wannier centers must interpolate between the secondary sites (at time \( K_y = 0 \)) and the non-secondary sites (at time \( K_y = \pi \)). One possible scenario is illustrated in Fig. (6.2-a). The conclusion is that \( C_1 \) is even.

It follows from Eq. (6.6), (6.1) and (6.2) that the product of all \( \mathcal{I} \) eigenvalues (over all occupied bands at every symmetric momenta) has the same parity as \( C_1 \).

Figure 6.3: The Wannier flow of a 2D insulator with both \( \mathcal{I} \) and TR symmetries. (a) This phase has a trivial TR-invariant; it is realized in the model Hamiltonian (6.7), with parameters \( m = 4.3, \delta = 0 \). (b) This phase has a nontrivial TR-invariant; it is realized in the same model, with \( m = 3, \delta = 0 \).
6.2.3 The Inversion- and Time-Reversal-Symmetric Wilson Loop

Our aim is to highlight distinctive features of Wilson loops with both \( I \) and time-reversal symmetries; we illustrate these features with a four-band model Hamiltonian:

\[
h(k) = (2 - m - \cos k_x - \cos k_y) \Gamma_{03} + \delta \sin k_y \Gamma_{12} \\
+ \sin k_x (\Gamma_{31} + \Gamma_{11}) + \sin k_y (\Gamma_{21} + \Gamma_{02}),
\]

with matrices \( \Gamma_{ij} \) defined as \( \sigma_i \otimes \tau_j \); \( \sigma_0, (\tau_0) \) is the identity in spin (orbital) space; \( \sigma_{i=1,2,3} \) (\( \tau_{i=1,2,3} \)) are Pauli matrices in spin (orbital) space. The Hamiltonian is \( I \)-symmetric:

\[
\Gamma_{03} h(k) \Gamma_{03} = h(-k).
\]

The Fermi energy is chosen so that there are two occupied bands in the ground state. We tabulate the \( I \) and \( W \)-eigenvalues for different choices of parameters \( m \) and \( \delta \) in Tab. 6.5. In this Section we set \( \delta = 0 \), so the Hamiltonian is also time-reversal symmetric (TRS): \( Th(k)T^{-1} = h(-k) \), with \( T = i\Gamma_{20}K \); \( K \) is the complex-conjugation operator. The two classes of TRS insulators are distinguished by a \( \mathbb{Z}_2 \) invariant \( \Xi \), which is the change in time-reversal polarization over half an adiabatic cycle; \( \Xi \) is odd for the nontrivial class. [3, 8–17, 78, 92–100] In Fig. (6.3-a) and (6.3-b), we have plotted the \( W_{k_y} \)-spectra for both \( \mathbb{Z}_2 \)-trivial (\( m = 4.3 \)) and nontrivial (\( m = 3 \)) phases respectively.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>( I ) eigenvalues</th>
<th>( W_{K_y} ) eigenvalues</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>( \delta )</td>
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</tr>
<tr>
<td>3</td>
<td>0</td>
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<td>1</td>
<td>((++))</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>((++))</td>
</tr>
<tr>
<td>4.3</td>
<td>0</td>
<td>((++))</td>
</tr>
</tbody>
</table>

Table 6.5: For various choices of the parameters \( m, \delta \) in the Hamiltonian (6.7), we write the corresponding (a) \( I \) eigenvalues at the four symmetric momenta and (b) the eigenvalues of \( W_{K_y} \).

As derived in Sec. 6.7, TRS imposes the following constraints on the \( W_{k_y} \) spectra:

(i) The sets of eigenvalues at \( \pm k_y \) are equal, \( i.e. \),

\[
\{ \exp i\vartheta_{k_y} \} = \{ \exp i\vartheta_{-k_y} \}.
\]
(ii) The $\mathcal{W}$'s at symmetric momenta satisfy

$$\mathcal{W}_{K_y}^{-1} = \Theta^{-1} \mathcal{W}_{K_y} \Theta,$$

(6.9)

with $\Theta$ an antiunitary operator that squares to $-I$. This implies that every eigenstate of $\mathcal{W}_{K_y}$ has a degenerate Kramer's partner. (i) and (ii) imply that if one Wannier center produces a Hall current $I_H$, its Kramer's partner produces a time-reversed current that cancels $I_H$. As shown in Ref. [71] and [78], the $\mathbb{Z}_2$ invariant may be extracted from Fig. (6.3) in the following manner: in the region $k_y \in [0, \pi]$, $\vartheta \in [-\pi, \pi]$, let us draw a constant-$\vartheta$ reference line at any value of $\vartheta$. If the Wannier trajectories intersect this reference line an odd number of times, the phase is nontrivial, and vice versa.

By imposing $\mathcal{I}$ symmetry as well, we arrive at the following conclusions:

(a) Due to $\mathcal{I}$ symmetry, the $\mathcal{W}_{K_y}$-spectra at $K_y = \{0, \pi\}$ consist of $\pm 1$ and complex-conjugate pairs; the additional constraint of Kramer's degeneracy implies that the spectra is composed of pairs of $[+1, +1]$, pairs of $[-1, -1]$ and complex-conjugate quartets $[\lambda \lambda^* \lambda^* \lambda^*]$. Since time-reversal and $\mathcal{I}$ commute, the two states in a Kramer's doublet must transform in the same representation under $\mathcal{I}$ – this limits the possible $\mathcal{I}$ eigenvalues in a TRS ground state.

(b) From (6.5) and (6.8) we derive

$$\{ \exp i\vartheta_{k_y} \} = \{ \exp -i\vartheta_{-k_y} \} = \{ \exp i\vartheta_{-k_y} \},$$

(6.10)

which indicates that the flow of the Wannier centers in one quadrant, say $\vartheta \in [0, \pi]$ and $k_y \in [0, \pi]$, determines the flow in the full range, $\vartheta \in [-\pi, \pi]$ and $k_y \in [-\pi, \pi]$, by reflections. This is illustrated in Fig. (6.3), where each quadrant is bounded by dotted lines.

### 6.2.4 Inversion-Protected Spectral Flow and the Relative Winding Number

The Chern insulator and the TRS topological insulator exhibit spectral flow in the $\mathcal{W}$-spectrum; the symmetries that protect spectral flow are, respectively, charge conservation
and time-reversal symmetry. In this Section, we report spectral flow of a third kind, which is protected by $\mathcal{I}$ symmetry alone. In our first example, we consider the eight-band model

$$h(k) = (-1 - \cos k_x - \cos k_y) \Theta_{030} + \sin k_x (\Theta_{310} + \Theta_{110})$$

$$+ \sin k_y (\Theta_{210} + \Theta_{020}) + 0.8 \sin k_x (\Theta_{311} + \Theta_{111}),$$

with matrices $\Theta_{ijk}$ defined as $\sigma_i \otimes \tau_j \otimes \gamma_k$; $\sigma_i = 1, 2, 3$ are Pauli matrices in spin space; for $i, j = \{1, 2, 3\}$, $\tau_i \otimes \gamma_j$ are products of Pauli matrices in a four-dimensional orbital space; $\sigma_0$ ($\tau_0 \otimes \gamma_0$) is the identity in spin (orbital) space. This Hamiltonian is $\mathcal{I}$-symmetric: $\Theta_{030} h(k) \Theta_{030} = h(-k)$, and time-reversal symmetric: $T h(k) T^{-1} = h(-k)$; here $T = i \Theta_{200} K$, and $K$ implements complex conjugation. The Fermi energy is chosen so that there are four occupied bands in the ground state. We tabulate the $\mathcal{I}$ and $\mathcal{W}$-eigenvalues in Tab. 6.6, and also plot the $\mathcal{W}_{k_y}$-spectrum in Fig. 6.4-a. With TRS, $C_1 = 0$. The change in time-reversal polarization over half an adiabatic cycle is 2 (even), hence the TR invariant is trivial. [8] Yet, Wannier trajectories interpolate across the full unit cell: $\vartheta \in [0, 2\pi)$. Let us softly break $\mathcal{I}$ symmetry, while maintaining TRS, with the perturbation: $0.4 \cos k_x \Theta_{022} + 0.4 \cos k_y \Theta_{112}$. As evidence that spectral flow persists only with $\mathcal{I}$ symmetry, we find in Fig. 6.4-b that...
the spectrum is now gapped.

<table>
<thead>
<tr>
<th>$\mathcal{I}$ eigenvalues</th>
<th>$W_{K_y}$ eigenvalues</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(0,0)$</td>
<td>$(\pi,0)$</td>
</tr>
<tr>
<td>$(0,\pi)$</td>
<td>$(\pi,\pi)$</td>
</tr>
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<td>$++$ $-$ $-$</td>
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<td>$++$ $-$ $-$</td>
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<tr>
<td>$+$ $+$ $+$ $+$ $+$ $+$</td>
<td>$++$ $-$ $-$</td>
</tr>
</tbody>
</table>

Table 6.6: For the Hamiltonian (6.11), we write the (a) $\mathcal{I}$ eigenvalues at the four symmetric momenta and (b) the eigenvalues of $W_{K_y}$.

$\mathcal{I}$-protected spectral flow is characterized by a nonzero relative winding number $W$, which is defined in the following way. Two Wannier trajectories are said to wind relative to each other if they (i) intersect the same primary site at a symmetric time $K_y$, then (ii) separate and intersect adjacent secondary sites half a period later ($K_y + \pi$). $W$ is defined as the number of stable pairs of relatively-winding trajectories. Our definition relies only on $\mathcal{I}$ symmetry, and does not depend on the presence or absence of any other symmetry. We outline a procedure to identify $W$:

(a) Count the number of Wannier trajectories that directly connect mid-bond and primary sites in the quadrant $\{\vartheta \in [0, \pi], k_y \in [0, \pi]\}$; call this number $n_1$. By a direct connection, we mean a smooth trajectory that flows without interruption. We consider three examples: in Fig. 6.5-a (blue) and 6.5-b (blue), $n_1 = 0$; $n_1 = 2$ in Fig. 6.4-a.

(b) Count the number of trajectories that directly connect mid-bond and primary sites in another quadrant $\{\vartheta \in [-\pi, 0), k_y \in [0, \pi]\}$; call this $n_2$. In all three examples, $n_1 = n_2$.

(c) $W$ is the minimum of $\{n_1, n_2\}$. We find that the insulator of Fig. 6.4-a has relative winding $W = 2$; $W = 0$ in the other two cases.

For each pair of relatively-winding trajectories, one of the pair ($\vartheta_1(k_y)$) has winding number $+1$ on the torus $\{\vartheta \in [-\pi, \pi], k_y \in [-\pi, \pi]\}$, and the other has winding $-1$. In principle, it is possible that $\vartheta_1(k_y)$ has winding $2n+1$ ($n \in \mathbb{Z}^+$), while its partner $\vartheta_2(k_y)$ has winding $-2n-1$. However, $n > 0$ implies that the trajectories $\vartheta_1(k_y)$ and $\vartheta_2(k_y)$ cross at a non-symmetric momentum ($k_y \neq \{0, \pi\}$); such degeneracies are not protected by symmetry - by a ground-state deformation that preserves both the energy gap and $\mathcal{I}$ symmetry, we may
turn crossings into anti-crossings and thus reduce $n$ to 0. Since $W$ is the number of stable relatively-winding pairs, we eliminate all such accidental degeneracies before carrying out the above procedure to identify $W$. All accidental degeneracies fall into two categories: (i) at non-symmetric momenta, there may be accidental crossings of two or more trajectories, as illustrated in Fig. 6.5-b (red). A slight deformation results in level repulsion, and turns crossings into anticrossings (Fig. 6.5-b (blue)). (ii) At symmetric momenta $\{0, \pi\}$, we rule out complex-conjugate-pair eigenvalues that are degenerate at either the primary or secondary site. In the example of Fig. 6.5-a (red), there is one such degeneracy at the primary site when $K_y = 0$, and another at the secondary site when $K_y = \pi$; upon perturbing the Hamiltonian, this degeneracy splits, as shown in Fig. 6.5-a (blue).

Figure 6.5: Figures in red provide two examples of accidental degeneracies. Upon a gap- and symmetry-preserving perturbation, these accidental degeneracies split, as shown in blue. These Wannier trajectories are calculated from 2D models; the Hamiltonians are not written explicitly. The model that describes the top two figures is a two-band model with $I$-eigenvalues equal to $\{+1, -1\}$ at all four inversion-invariant momenta. These are mapped to complex-conjugate $W$-eigenvalues $[\lambda, \lambda^*]$, along both $k_y = 0$ and $k_y = \pi$; cf. Sec. 6.1.2. $\lambda$ may vary in the interval $[1, -1]$, by continuous reparametrization of the Hamiltonian that maintains both energy gap and symmetry.

Let us derive a sufficient condition for relative winding, and simultaneously relate $W$,
Figure 6.6: Schematic illustrations of Wannier trajectories for eight occupied bands, where $N_d = 4$. (a) All four red trajectories wind with center-of-mass motion, thus $C_1 = -4$, $W = 0$. (b) One pair of red trajectories relatively wind, so $C_1 = -2$, $W = 1$. (c) Both pairs of red trajectories relatively wind, hence $C_1 = 0$, $W = 2$.

$C_1$ and the eigenvalues of $W$ at constant $K_y = \{0, \pi\}$. We define $N_{(+1)}(K_y)$, $N_{(-1)}(K_y)$ and $N_{(cc)}(K_y)$ as the number of $+1$, $-1$ and complex-conjugate-pair eigenvalues of $W_{K_y}$, respectively; $N_{(+1)}(K_y)+N_{(-1)}(K_y)+N_{(cc)}(K_y) = n_{occ}$, the number of occupied bands. These quantities constrain the possible Wannier trajectories that interpolate between $K_y = 0$ and $\pi$, and by implication they also constrain the possible topological invariants: $W$, $C_1$ and $\Xi$.

Define $N_d$ as the maximum of two quantities:

$$N_d = \max \{ N_{(-1)}(\pi) - N_{(-1)}(0) - N_{(cc)}(0),$$

$$N_{(-1)}(0) - N_{(-1)}(\pi) - N_{(cc)}(\pi) \}.$$  \hfill (6.12)

If $N_d > 0$, there are $N_d$ trajectories that directly connect the secondary site (at $K_y$) and the primary site (at $K_y + \pi$). Of these $N_d$ trajectories, one or more pairs may relatively wind, and the rest wind with center-of-mass motion, thus contributing to the Chern number $C_1$.

The parity of $C_1$ is constrained as in (6.6). A sufficient condition for relative winding is that $|C_1| < N_d$, in which case $2W = N_d - |C_1|$. If $|C_1| \geq N_d$, then $W = 0$. In Fig. 6.6, we schematically illustrate three cases where $N_d = N_{(-1)}(0) - N_{(-1)}(\pi) - N_{(cc)}(\pi) = 7 - 1 - 2 = 4$, i.e., there are four trajectories (in red) that directly connect the secondary site (at $\pi$) and the primary site (at $0$). There are five ways to split four trajectories into center-of-mass and relative windings: $N_d = |C_1| + 2W = | -4 | + 2(0) = | -2 | + 2(1) = |0| + 2(2) = |2| + 2(1) = |4| + 2(0)$. We illustrate the first three cases in Fig. 6.6-a, b, and c respectively. For $I$- and time-reversal-symmetric ($I+\text{TRS}$) insulators, $C_1 = 0$, hence the relative winding is related
to $N_d$ through: $2W = N_d$.

<table>
<thead>
<tr>
<th>$U(1)$</th>
<th>TRS</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W &gt; 0$</td>
<td>$2W +</td>
</tr>
<tr>
<td>$W = 0$</td>
<td>$</td>
</tr>
</tbody>
</table>

Table 6.7: Relations between relative winding $W \in \mathbb{Z}^\geq$, the Chern number $C_1 \in \mathbb{Z}$, the TR invariant $\Xi \in \mathbb{Z}_2$, and eigenvalues of the Wilson loop at symmetric momenta. Columns: $U(1)$ denotes a generic insulator with charge-conservation symmetry; TRS denotes a time-reversal symmetric insulator. $N_d$ is defined in Eq. (6.12).

Relative Winding of Insulators with both Inversion and Time-Reversal Symmetries

In this Section we study the relative winding of insulators with both $\mathcal{I}$ and TRS (I+TRS); we shall relate the relative winding $W$ with the TR invariant $\Xi$. While both $W$ and $\Xi$ characterize Wannier trajectories with no center-of-mass motion, they differ in many important respects. For I+TRS insulators with nonzero relative winding, the parity of $W$ determines the TR invariant: $\Xi = W \mod 2$; $\Xi$ is odd in the nontrivial class. To prove this, we apply the rule: modulo 2, $\Xi$ equals the number of Wannier trajectories that intersect a constant-$\vartheta$ reference line. [71] With I+TRS, only one quadrant, e.g. $\{ \vartheta \in [0, \pi], k_y \in [0, \pi] \}$, is independent. In the rest of this section, we denote coordinates in this quadrant by $(\vartheta, k_y)$. Two cases are possible: (i) $W$ number of trajectories directly connect points $(\vartheta, k_y) = (\pi, 0)$ and $(0, \pi)$, or (ii) $W$ trajectories connect $(\pi, \pi)$ and $(0, 0)$. If $n_{occ} = 2W$, there are exactly $W$ intersections with the reference line, hence $\Xi = W \mod 2$. If $n_{occ} > 2W$, it is possible in case (i) that: (i-a) an extra trajectory connects $(0, 0)$ and $(0, \pi)$, (i-b) a trajectory connects $(\pi, 0)$ and $(\pi, \pi)$, (i-c) if there exists a complex-conjugate quartet $[\lambda_1 \lambda_1^* \lambda_1^*]$ in the spectrum of $W_{K_y=0}$, a pair of trajectories may connect $(0, \pi)$ with the complex-conjugate site at $(\lambda_1, 0)$, and (i-d) if there exists a complex-conjugate quartet $[\lambda_2 \lambda_2^* \lambda_2^*]$ in the spectrum of $W_{K_y=\pi}$, a pair of trajectories may connect $(\pi, 0)$ with the complex-conjugate site $(\lambda_2, \pi)$. In
all scenarios, these extra trajectories intersect an even number of times with the reference line – the parity of the number of intersections is decided by $W$ alone. The proof is complete.

While only the parity of $W$ matters to the $\mathbb{Z}_2$ classification under TRS, $W$ provides a $\mathbb{Z}^\geq$ classification under $I$ symmetry, and hence a more complete characterization. This distinction may be understood from a stability analysis of the Wannier centers. Since Kramer’s degeneracy is two-fold, four or more Wannier centers generically experience level repulsion. Consider for example the $W = 2$, I+TRS model of Fig. 6.4-a. Sitting at the primary site (at $K_y = \pi$) are four Wannier centers which are constrained by $I$-symmetry – they do not experience level repulsion. If we now break $I$-symmetry while preserving TRS, these four Wannier centers destabilize and split to form two pairs of Kramer’s doublets, thus breaking spectral flow; see Fig. 6.4-b.

For I+TRS insulators with zero relative winding, it is possible that spectral flow is completely absent and the insulator is trivial. However, an I+TRS insulator with four or more occupied bands may have a nontrivial TR invariant without relative winding. To distinguish these two cases, we look to the indices $N_{(-1)}(0)$ and $N_{(-1)}(\pi)$. Since $W = 0$, all $N_{(-1)}(K_y)$ Wannier centers that originate from the secondary site (at $K_y$) must flow to either a complex-conjugate site or a secondary site (at $K_y + \pi$). By conservation of trajectories, $N_{(-1)}(K_y) - N_{(-1)}(K_y + \pi)$ number of trajectories must connect the secondary site (at $K_y$) to complex-conjugate sites (at $K_y + \pi$); here we have assumed $N_{(-1)}(K_y) > N_{(-1)}(K_y + \pi)$. Since $C_1 = 0$, we know from (6.6) that $N_{(-1)}(K_y) - N_{(-1)}(K_y + \pi)$ is even – within one quadrant, e.g., $\{\theta \in [0, \pi], k_y \in [K_y, K_y + \pi]\}$, $(N_{(-1)}(K_y) - N_{(-1)}(K_y + \pi))/2$ number of trajectories connect the secondary site (at $K_y$) to complex-conjugate sites (at $K_y + \pi$). Two cases arise: (i) if $(N_{(-1)}(K_y) - N_{(-1)}(K_y + \pi))/2$ is odd, there must be at least one other trajectory that interpolates between $K_y$ and $K_y + \pi$. Then the sum of all trajectories that connect to complex-conjugate sites is even, as required by Kramer’s degeneracy. Hence, TRS enforces a zig-zag pattern of Wannier flows, as illustrated schematically in Fig 6.7-a.
and -b. (ii) For even \((N_{-1}(K_y) - N_{-1}(K_y + \pi))/2\), Kramer’s degeneracy is satisfied without additional trajectories, and the resultant Wannier flows are gapped, as in Fig. 6.7-c and -d. Therefore,

\[
\Xi = \frac{1}{2} \left( N_{-1}(0) - N_{-1}(\pi) \right) \mod 2 \nonumber
\]

\[
= \frac{1}{2} N_d \mod 2; \quad (6.13)
\]

for the last equality, we applied the definition of \(N_d\) in Eq. (6.12) and that \(N_{(co)}(K_y)\) is a multiple of four; c.f. Sec. 6.2.3. The relation (6.13) applies to I+TRS insulators with \(W > 0\) as well, since we have proven \(\Xi = W \mod 2\) in this Section, and previously identified \(2W = N_d\) in Sec. 6.2.4. The relations between \(\Xi\), \(W\) and \(N_d\) are summarized in Tab. 6.7.

Consider for example the eight-band model:

\[
h(k) = (-2 - \cos k_x - \cos k_y) \Theta_{033} + \frac{4}{5} \cos k_y \Theta_{001}
\]

\[
+ 5 \sin k_x (\Theta_{113} + \Theta_{313}) - \frac{3}{2} \sin k_y (\Theta_{020} + \Theta_{210})
\]

\[
+ (6 \sin k_x + \frac{7}{2} \sin k_y) (\Theta_{023} + \Theta_{213}) + \Theta_{030}, \quad (6.14)
\]

with matrices \(\Theta_{ijk}\) defined in (6.11). This Hamiltonian has the same symmetries as that in (6.11), namely \(I\) and TRS, and the ground state is defined to be the four lowest-energy wavefunctions.
bands. We tabulate the $\mathcal{I}$ and $\mathcal{W}$-eigenvalues in Tab. 6.8. As illustrated in Fig. 6.8-a, the relative winding is trivial, but partner-switching occurs with help from the complex-conjugate quartet at $K_y = 0$. In this $W = 0$ model, spectral flow is protected by TRS alone. As evidence, we deform the Hamiltonian with a TRS-breaking term, $\Delta h(k) = 8 \sin k_x (\Theta_{022} + \Theta_{120} + \Theta_{121}) + 2 \sin k_y \Theta_{123}$, which preserves both the energy gap and $\mathcal{I}$ symmetry. As illustrated in Fig. 6.8-b, Kramer’s degeneracy is now lifted – the quartet $[\lambda\lambda^*\lambda^*\lambda^*]$ at $K_y = 0$ splits into two separate doublets $[\lambda_1 \lambda_1^*], [\lambda_2 \lambda_2^*]$. This contrasts with a previous example, where we broke TRS in a $\Xi$-nontrivial phase; as shown in Fig. 6.1-b, the resultant $\mathcal{W}$-spectrum is not gapped, due to a nonzero relative winding.

<table>
<thead>
<tr>
<th>$\mathcal{I}$ eigenvalues</th>
<th>$\mathcal{W}_{K_y}$ eigenvalues</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 0)</td>
<td>$K_y = 0$</td>
</tr>
<tr>
<td>$(\pi, 0)$</td>
<td>$K_y = \pi$</td>
</tr>
<tr>
<td>$(0, \pi)$</td>
<td>$\lambda_1 \lambda_1^*$</td>
</tr>
<tr>
<td>$(\pi, \pi)$</td>
<td>$+ + --$</td>
</tr>
<tr>
<td>+ + --</td>
<td>$+ + --$</td>
</tr>
<tr>
<td>+ + --</td>
<td>$+ + --$</td>
</tr>
<tr>
<td>$\lambda_2 \lambda_2^*$</td>
<td>$K_y = 0$</td>
</tr>
<tr>
<td>$K_y = \pi$</td>
<td>$K_y = \pi$</td>
</tr>
</tbody>
</table>

Table 6.8: For the Hamiltonian (6.14), we write the (a) $\mathcal{I}$ eigenvalues at the four symmetric momenta and (b) the eigenvalues of $\mathcal{W}_{K_y}$.

Figure 6.8: (a) An $\mathcal{I}$-symmetric phase with zero relative winding; spectral flow persists due to TRS alone. This is the ground state of Hamiltonian (6.14). (b) Spectral flow is interrupted with a TRS-breaking perturbation.
6.3 Analytic Properties of the Sewing Matrix and Constraints on the Wilson Loop due to Inversion Symmetry

Let us employ the bra-ket notation that is introduced in Sec. 2.3. Inversion symmetry constrains the Hamiltonian as \( \varphi h(k) \varphi = h(-k) \), as shown in Sec. 1.2. This implies that the occupied eigenstates \( U^m_k \) at \( \pm k \) are related through inversion by a \( U(n_{\text{occ}}) \) ‘sewing matrix’ \( B_k \):

\[
[U^m_{-k}]_\alpha = \sum_{n=1}^{n_{\text{occ}}} \sum_{\beta} B^{m*}_{k\alpha\beta} [U^n_k]_\beta.
\]

(6.15)

Here, \( m, n \) are indices that label the occupied bands. Alternatively, \( B^{m*}_{k\alpha\beta} = [U^m_{-k}]_\alpha \varphi_{\alpha\beta} [U^n_k]_\beta = \langle U^m_k | \varphi | U^n_k \rangle \). We define the inversion-invariant momenta \( k^{\text{inv}} \) as satisfying \( -k^{\text{inv}} = k^{\text{inv}} + G(k^{\text{inv}}) \) for some reciprocal lattice vector \( G \). Implicit in the Wilson loop is the periodic gauge condition (3.29), from which we find

\[
B^{m*}_{k\alpha\beta} = \langle U^m_{k^{\text{inv}}} | V(G(k^{\text{inv}})) \varphi | U^n_{k^{\text{inv}}} \rangle.
\]

For an inversion-symmetric unit cell, it follows that \( V(G) \varphi^{-1} = V(-G) \), and hence \((V(G(k^{\text{inv}}))) \varphi)^2 = \varphi^2 = I\), thus the inversion operator \( V(G(k^{\text{inv}})) \varphi \) has eigenvalues \( \pm 1 \). It follows from \( \varphi h(k) \varphi = h(-k) \) that \([h(k^{\text{inv}}), V(G(k^{\text{inv}})) \varphi] = 0\), thus it is possible to find a basis in which \( U^n_{k^{\text{inv}}} \) are eigenstates of \( V(G(k^{\text{inv}})) \varphi \). Then \( B_{k^{\text{inv}}} \) is a diagonal matrix with diagonal elements equal to the \( I \) eigenvalues of \( U^n_{k^{\text{inv}}} \). In deriving the gauge-invariant \( W \)-eigenspectrum, we will employ such a convenient gauge. We prove that \( B_k \) is unitary.

Let us label the unoccupied bands by the primed index \( m' = n_{\text{occ}} + 1, \ldots, n_{\text{tot}} \). If the ground state is insulating, i.e., \( \langle U^m_k | \varphi | U^n_k \rangle = 0 \) for all \( n \) occupied bands and all \( m' \) unoccupied bands,

\[
\sum_{m=1}^{n_{\text{occ}}} B^{m*}_{k} B^{m'}_{k} = \sum_{m=1}^{n_{\text{occ}}} \langle U^m_k | \varphi | U^n_k \rangle \langle U^m_k | \varphi | U^n_k \rangle^{*} = \sum_{m=1}^{n_{\text{tot}}} \langle U^m_l | \varphi | U^n_k \rangle \langle U^m_k | \varphi | U^n_k \rangle = \delta^n_l.
\]

(6.16)

In the second equality, we have used the identity: \( \langle U^m_k | \varphi | U^n_k \rangle = 0 \); the third equality required the completeness relation. Furthermore, the Hermicity of the inversion operation
\[ \varphi \] implies \( B_k = [B_k]^{-1} \). Applying (6.15) and \( \varphi^2 = I \), we derive the following condition for a Wilson line between two infinitesimally-separated momenta \( k^{(1)} \) and \( k^{(2)} \):

\[ W_{mn}^{\pi \to -\pi} = B_{\pi}^{mr} \ W_{\pi \to -\pi}^{rs} B_{\pi}^{ns} = B_{\pi}^{mr} \ W_{\pi \to -\pi}^{rs} B_{\pi}^{ns} = B_{\pi}^{mr} \ W_{\pi \to -\pi}^{rs} B_{\pi}^{ns} [B_{\pi}^{-1}]^T. \quad (6.19) \]

Here we have used the identities (2.29) and \( B_{\pi}^{k_{inv}} = B_{\pi}^{k_{inv}}. \) (6.19) informs us that \( W \) is equivalent to its Hermitian adjoint through a unitary transformation, \( i.e. \), the set of \( W \)-eigenvalues is equal to its complex conjugate:

\[ \{ \exp i\theta \} = \{ \exp -i\theta \}. \quad (6.20) \]

Let us derive a second useful identity. The Wilson loop along \( \mathcal{L} \) may be decomposed into two Wilson lines that each connect two symmetric momenta: \( W(\mathcal{L}) = W_{\pi \to 0} W_{0 \to -\pi}. \) Up to a change in orientation, \( W_{\pi \to 0} \) is mapped to \( W_{0 \to -\pi} \) by an inversion \( k \to -k \). Applying (6.18),

\[ W_{\pi \to -\pi}^{mn} = W_{\pi \to 0}^{ml} W_{0 \to -\pi}^{ln} = B_{\pi}^{mr} [W_{\pi \to -\pi}^{rs}] B_{0}^{sl} W_{0 \to -\pi}^{ln}. \quad (6.21) \]
6.4 Case Studies of the 1D Inversion-Symmetric Insulator

6.4.1 Case Study: 1 Occupied Band

With one occupied band, there is only one Wannier center per unit cell. In each unit cell, the Wannier center can only be at a primary site or at a secondary site; only these spatial configurations in a periodic lattice are invariant under inversion. If the Bloch waves at \( k = 0 \) and \( \pi \) transform under different representations of \( \mathcal{I} \), \( \mathcal{W} = -1 \). Proof: We shall employ notation that is defined in (6.21). Being unitary, \( \mathcal{W}_{0\rightarrow-\pi} \) must be of the form \( \exp(i\vartheta) \).

(6.21) informs us that \( \mathcal{W}(L) = B_\pi \exp(-i\vartheta) B_0 \exp(i\vartheta) = B_\pi B_0 \), which is a product of the \( \mathcal{I} \) eigenvalues of the sole occupied band at \( k = 0 \) and \( \pi \). The proof is complete. This result can be verified by a model tight-binding Hamiltonian

\[
h(k) = -(\alpha + \cos k) \tau_3 + \sin k \tau_2,
\]

(6.22)

with \( \tau_i \) defined as Pauli matrices in orbital space. This Hamiltonian has an \( \mathcal{I} \) symmetry: \( \tau_3 h(k) \tau_3 = h(-k) \); the insulator is trivial when \( \alpha > 1 \), and nontrivial when \(-1 < \alpha < 1\).

6.4.2 Case Study: 2 Occupied Bands

For \( \mathcal{I} \)-symmetric insulators with two occupied bands, \( \mathcal{W} \) is a \( 2 \times 2 \) matrix; our case study captures many qualitative features of larger-dimensional \( \mathcal{W} \)'s. We assume a general form for \( \mathcal{W}_{0\rightarrow-\pi} \) that satisfies unitarity:

\[
\mathcal{W}_{0\rightarrow-\pi} = e^{i\alpha} \begin{pmatrix} c & d \\ -d^* & c^* \end{pmatrix}; \quad |c|^2 + |d|^2 = 1.
\]

(6.23)

Inserting (6.23) into (6.21), we arrive at \( \mathcal{W}(L) = \)

\[
\begin{pmatrix}
\xi_\pi^1 (|c|^2 \xi_0^1 + |d|^2 \xi_0^2) & c^* d \xi_\pi^1 (\xi_0^1 - \xi_0^2) \\
c d^* \xi_\pi^2 (\xi_0^1 - \xi_0^2) & \xi_\pi^2 (|c|^2 \xi_0^2 + |d|^2 \xi_0^1)
\end{pmatrix},
\]

(6.24)

where \( \xi_k^{1,2} \) are diagonal elements of the sewing matrix \( B_k \). We exhaust the possible \( \mathcal{I} \) eigenvalues \( \{ \xi_k \} \), solve the characteristic equations and derive the \( \mathcal{W} \) spectra. Our results are tabulated in Tab. 6.2.
Cases (i)-(iii) of Tab. 6.2 may be summarized as: if the $I$ eigenvalues of occupied bands at either $k = 0$ or $\pi$ are identical, *i.e.*, if either sewing matrix $B_0$ or $B_\pi$ is proportional to the identity, then the $W$-spectrum comprises only $\pm 1$ eigenvalues; its eigenvalues are the diagonal elements of the product $B_0 B_\pi$.

In case (iv) of Tab. 6.2, we encounter (a) occupied bands with nonidentical $I$ eigenvalues at both $k = 0$ and $\pi$, and (b) a complex-conjugate pair of $W$-eigenvalues ($\lambda \lambda^*$): a pair of Wannier centers are positioned equidistantly on opposite sides of each primary site. The exact position is not determined by symmetry; this arbitrariness reflects the range in this equivalence class of $I$-symmetric insulators, *i.e.*, it is possible to tune the Hamiltonian and sweep the interval of allowed $\lambda$ while preserving both the insulating gap and $I$ symmetry. This implies that case (iv) is trivial. Why? Let us tune the Hamiltonian to a limit in which bands of identical representation are fully coupled, *i.e.*, the positive-$I$ (negative-$I$) band at $k = -\pi$ adiabatically evolves into the positive-$I$ (negative-$I$) at 0, through the Wilson line $W_{0\rightarrow-\pi}$. For example, if $\xi^1_0 = \xi^2_\pi = -\xi^1_\pi = -\xi^2_0$, the two $W$-eigenvalues are $|d|^2 - |c|^2 \pm 2i|c||d|$. Tuning $|c| \rightarrow 0$ and $|d| \rightarrow 1$ effectively decouples the two-band $W$ into two one-band $W$’s; each Abelian $W$ connects bands of the same representation between $k = 0$ and $\pi$, hence each contributes $+1$ to the spectrum, and $W \rightarrow I$. As discussed in the Introduction, if $W$ is tunable to the identity, then the insulator is in the same equivalence class as the atomic insulator, hence we conclude that case (iv) is trivial.

In contrast with complex-conjugate-pair $W$-eigenvalues, protected $-1$ eigenvalues obstruct $W$ from being tuned to the identity. The nontrivial insulators are cases (ii) and (iii) of Tab. 6.2, which have one and two $-1$ eigenvalues respectively. We distinguish between case (iii) and the degenerate limit of case (iv), in which $W \rightarrow -I$; this is the limit in which bands of identical representation are fully decoupled, *i.e.*, the positive-$I$ (negative-$I$) band at $k = -\pi$ adiabatically evolves into the negative-$I$ (positive-$I$) at 0. In case (iii), the equality $W = -I$ is robust against gap- and symmetry-preserving transformations of the ground-state, while this is not true in case (iv).
Table 6.9: A model of an $I$-symmetric ground state with two occupied bands: for various choices of the parameters $\alpha, \beta$ in the Hamiltonian (6.25), we write the corresponding $I$ and $W$-eigenvalues.

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>$I$ eigenvalues</th>
<th>$W$ spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>$\beta$</td>
<td>$\pi$</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>$(++)$</td>
</tr>
<tr>
<td>1.5</td>
<td>0</td>
<td>$(+-)$</td>
</tr>
<tr>
<td>1.5</td>
<td>-1.5</td>
<td>$(-+)$</td>
</tr>
<tr>
<td>1.5</td>
<td>1.5</td>
<td>$(+-)$</td>
</tr>
</tbody>
</table>

Let us verify our results in Tab. 6.2 with the model, tight-binding Hamiltonian

$$h(k) = -\Gamma_{03} + 0.1 \Gamma_{13} + (\Gamma_{21} + \Gamma_{31}) \sin k$$

$$+ \frac{1}{2} \left( \alpha (\Gamma_{30} + \Gamma_{03}) + \beta (\Gamma_{30} - \Gamma_{03}) \right) \cos k,$$

(6.25)

with matrices $\Gamma_{ij}$ defined as $\sigma_{i} \otimes \tau_{j}$; $\sigma_{0}$ ($\tau_{0}$) is the identity in spin (orbital) space; $\sigma_{i=1,2,3}$ ($\tau_{i=1,2,3}$) are Pauli matrices in spin (orbital) space. The Hamiltonian is $I$-symmetric: $\Gamma_{03} h(k) \Gamma_{03} = h(-k)$. The Fermi energy is chosen so that there are two occupied bands in the ground state. We tabulate the $W$ spectra for various choices of the parameters $\alpha$ and $\beta$ in Tab. 6.9.

### 6.5 Proof of mapping between $I$ and $W$ eigenvalues

We employ notation that has been defined in Sec. 6.1.2: $n_{(\pm)}(k^{\text{inv}})$, FBOP, $k_{s}, \xi_{s}, n_{s}$. As defined in Eq. (6.15), $B_{k}$ is a $U(n_{\text{occ}})$ sewing matrix linking bands at $\pm k$ through $I$. At symmetric momenta $k^{\text{inv}}$, a gauge is chosen in which $B_{k^{\text{inv}}}$ is a diagonal matrix with elements \(\{\xi_{1}(k^{\text{inv}}), \xi_{2}(k^{\text{inv}}), \ldots, \xi_{n_{\text{occ}}}(k^{\text{inv}})\}\) equal to the $I$ eigenvalues at $k^{\text{inv}}$. At momentum $k_{s}$, we pick a convention that the fewest bands of one parity (FBOP) are indexed by $m = 1, 2, \ldots, n_{s}$ and the rest of the bands at $k_{s}$ are indexed by $m = n_{s} + 1, \ldots, n_{\text{occ}}$. We evaluate the Wilson loop $W$ over a path that begins at $k_{s} - \pi$, sweeps the interval $[k_{s} - \pi, k_{s} + \pi]$ and ends at $k_{s} + \pi$; the $W$-spectrum is independent of the base point, as shown in Sec. 2.4. In the rest of the section, we simplify notation and assume that $W = W_{k_{s} + \pi - k_{s} - \pi}$. Let us reproduce a result presented in (6.21): $W = B_{k_{s} + \pi} Z_{B_{k_{s}}} Z$, with $Z$ defined as the Wilson
line $W_{k_s+k_s-\pi}; Z^{-1} = Z^\dagger$. Let us define $Y$ as the $n_{\text{occ}} \times n_{\text{occ}}$ matrix

$$Y = \frac{1}{2} \left( I + \xi_s B_{\pi+k_s} W \right). \quad (6.26)$$

Since $B_{\pi+k_s}^2 = I$, the matrix elements of $Y$ are

$$Y_{ij} = \frac{1}{2} (I + \xi_s Z^\dagger B_{k_s} Z)^{ij} = \sum_{l=1}^{n_s} Z^*_l Z_{lj}. \quad (6.27)$$

Here we have applied the unitarity condition $Z^\dagger Z = I$ to express

$$[Z^\dagger B_{k_s} Z]_{ij} = \sum_{a=1}^{n_{\text{occ}}} \xi_a(k_s) Z^*_a Z_{aj} = -\xi_s(\delta_{ij} - 2 \sum_{b=1}^{n_s} Z^*_b Z_{bj}). \quad (6.28)$$

We deduce from (6.27) that $Y$ is a rank-$n_s$ projection matrix. If $n_s = 0$, $Y$ is the zero matrix. We define $\bar{Y}_{\alpha_1\alpha_2...\alpha_m}$ as $m \times m$ submatrices in $Y$ that lie on the intersections of rows numbered by $\{\alpha_1, \alpha_2, ..., \alpha_m\}$ with columns numbered by $\{\alpha_1, \alpha_2, ..., \alpha_m\}$. For example, $\bar{Y}_1 = \sum_{a=1}^{n_s} Z^*_a. Z_{1a}$, and

$$\bar{Y}^{23} = \begin{pmatrix} \sum_{a=1}^{n_s} Z^*_{a,2} Z_{a,2} & \sum_{a=1}^{n_s} Z^*_{a,3} Z_{a,3} \\ \sum_{a=1}^{n_s} Z^*_{a,3} Z_{a,2} & \sum_{a=1}^{n_s} Z^*_{a,3} Z_{a,3} \end{pmatrix}. \quad (6.29)$$

The determinant of a $m \times m$ submatrix $\bar{Y}$ is also called the $m \times m$ minor of $Y$. According to a well-known theorem in linear algebra, the rank of a matrix is equal to the largest integer $r$ for which a nonzero $r \times r$ minor exists, therefore $\det \bar{Y}^{\alpha_1\alpha_2...\alpha_m} = 0$ if $m > n_s$. Applying (6.26), the characteristic equation $\det[\lambda I - W] = 0$ is equivalent to

$$0 = \det[\xi_s B_{k_s+\pi}] \det[\lambda I - W] \quad = \det[(-\xi_s \lambda B_{k_s+\pi} - I) + 2Y] \quad (6.30)$$

We claim that the determinant in the second line of (6.30) is equal to a polynomial in $\lambda$ of order $2n_s$, multiplied by the factor $(-\xi_s \lambda-1)^{[n_+(k_s+\pi)-n_s]} (\xi_s \lambda-1)^{[n_-(k_s+\pi)-n_s]}$, where $n_+(k_s+\pi)$ and $n_-(k_s+\pi)$ is the number of positive-$I$ (negative-$I$) bands at $k_s + \pi$. Upon proving this claim, we deduce that there are $(n_+(k_s+\pi)-n_s)$ number of $-\xi_s$ $W$-eigenvalues and $(n_-(k_s+\pi)-n_s)$ number of $+\xi_s$ $W$-eigenvalues. Furthermore, we apply a result.
presented in (6.20): the $W$-eigenvalues can either be $\pm 1$ or form complex-conjugate pairs $\lambda, \lambda^*$. Thus, the zeros of the polynomial $R(\lambda)$ correspond to $n_s$ complex-conjugate pairs of eigenvalues.

**Proof:**

We define $\lambda_i = -\xi_s \xi_i(k_s + \pi) \lambda$. By a binomial-like expansion, we express the characteristic equation as:

$$0 = \sum_{m=0}^{n_{\text{occ}}} 2^m \sum_{\{\alpha_1, \alpha_2, \ldots, \alpha_m\}} \det Y^{\alpha_1 \alpha_2 \ldots \alpha_m} \prod_{i=1; i \neq \alpha_1, \alpha_2, \ldots, \alpha_m}^{n_{\text{occ}}} (\lambda_i - 1). \quad (6.31)$$

The sum $\sum_{\{\alpha_1, \alpha_2, \ldots, \alpha_m\}}$ runs over the $n_{\text{occ}}$ choose $m$ combinations of the indices $\{\alpha_1 \ldots \alpha_m\}$.

An example of the characteristic equation for an insulator with 4 occupied bands is

$$0 = (\lambda_1 - 1)(\lambda_2 - 1)(\lambda_3 - 1)(\lambda_4 - 1)$$

$$+ \left[ 2 Y^1(\lambda_2 - 1)(\lambda_3 - 1)(\lambda_4 - 1) + 8 \det [Y^{123}] (\lambda_4 - 1) + \text{comb. 1} \right]$$

$$+ \left[ 4 \det [Y^{12}] (\lambda_3 - 1)(\lambda_4 - 1) + \text{comb. 2} \right] + 16 \det [Y^{1234}] \quad (6.32)$$

where $[f(1234) + \text{comb. 1}] = f(1234) + f(4123) + f(3412) + f(2341)$ and $[f(1234) + \text{comb. 2}] = f(1234) + f(1324) + f(1423) + f(2314) + f(2413) + f(3412)$. Applying the rank-minor theorem, only the first $n_s + 1$ terms in (6.31) are nonzero:

$$0 = \sum_{m=0}^{n_s} 2^m \sum_{\{\alpha_1, \alpha_2, \ldots, \alpha_m\}} \det Y^{\alpha_1 \alpha_2 \ldots \alpha_m} \prod_{i=1; i \neq \alpha_1, \alpha_2, \ldots, \alpha_m}^{n_{\text{occ}}} (\lambda_i - 1). \quad (6.33)$$

Let us organize this expansion. We first consider a term in (6.33) with a particular combination of $m$ band indices given by the set $\{\alpha_1 \ldots \alpha_m\}$ in the superscript of $Y$. Each band index $\alpha_i$ has a corresponding $I$ eigenvalue $\xi_{\alpha_i}$ at $k = k_s + \pi$; in this set we may define $m_+ (m_-)$ as the number of positive (negative) $I$ eigenvalues in the set $\{\xi_{\alpha_1}(k_s + \pi) \ldots \xi_{\alpha_m}(k_s + \pi)\}$; note $m_+ + m_- = m$. The presence of each band $\alpha_i$ in this set implies that a factor of $(-\xi_s \xi_{\alpha_i}(k_s + \pi) \lambda)$ is absent in the product $\prod_{i=1; i \neq \alpha_1, \alpha_2, \ldots, \alpha_m}^{n_{\text{occ}}} (\lambda_i - 1)$. In the remainder of this proof, we use the convention that $\alpha_i$ ($\beta_i$) are positive-$I$ (negative-$I$) band indices at $\pi + k_s$. We may organize the expansion by collecting terms with the same $m_+$:

$$0 = \sum_{m=0}^{n_s} 2^m \sum_{m_+=0}^{m} (-\xi_s \lambda - 1)^{n_{\text{occ}}(k_s+\pi)-m_+} (\xi_s \lambda - 1)^{n_{\text{occ}}(k_s+\pi)-m+m_+} S_{m_+, m-m_+} \quad (6.34)$$
with $S_{x,y}$ defined as the sum of all minors $\det \bar{Y}^{\alpha_1...\alpha_{m_+}\beta_1...\beta_{m_-}}$ with $m_+ = x$ and $m_- = y$:

$$S_{x,y} = \sum_{\{\alpha_1...\alpha_x \beta_1...\beta_y\}} \det \bar{Y}^{\alpha_1...\alpha_x \beta_1...\beta_y}. \quad (6.35)$$

By definition, there are $n_{(+)}(k_s + \pi) (n_{(-)}(k_s + \pi))$ number of positive-$I$ (negative-$I$) bands at $k_s + \pi$, hence the sum $\sum_{\{\alpha_1...\alpha_x \beta_1...\beta_y\}}$ runs over $n_{(+)}(k_s + \pi)$ choose $x$ combinations of positive-$I$ bands, multiplied by $n_{(-)}(k_s + \pi)$ choose $y$ combinations of negative-$I$ bands. As the form of (6.34) suggests, nonzero terms in the expansion have values of $m_+$ ranging from a minimum of 0 to a maximum of $n_s$. That the expansion (6.33) includes nonzero terms with $m_+ = n_s, m_- = 0$ and nonzero terms with $m_+ = 0, m_- = n_s$ is a consequence of our construction: by definition of FBOP and $n_s$, both $n_{(+)}(k_s + \pi)$ and $n_{(-)}(k_s + \pi) \geq n_s$. We observe that:

(i) Terms in the expansion with $m_+ = n_s, m_- = 0$ are proportional to $(-\xi_s \lambda^{-1})^{[n_{(+)}(k_s+\pi)-n_s]}$ because $n_s$ factors of $(-\xi_s \lambda \xi_{\alpha_i}(k_s + \pi)-1)$ with $\xi_{\alpha_i} = +1$ are removed from the product $\Pi(\lambda^{-1})$. All other terms in the expansion have greater powers of $(-\xi_s \lambda^{-1})$.

(ii) Similarly, terms in the expansion with $m_+ = 0, m_- = n_s$ are proportional to

$$(-\xi_s \lambda^{-1})^{[n_{(-)}(k_s+\pi)-n_s]} \quad (6.36)$$

and all other terms in the expansion have greater powers of $(-\xi_s \lambda^{-1})$.

(i) and (ii) imply that the common factor of all terms in the expansion is

$$(-\xi_s \lambda^{-1})^{[n_{(+)}(k_s+\pi)-n_s]} \cdot (-\xi_s \lambda^{-1})^{[n_{(-)}(k_s+\pi)-n_s]} \quad (6.37)$$

The characteristic equation is thus expressible as

$$0 = (-\xi_s \lambda^{-1})^{[n_{(+)}(k_s+\pi)-n_s]} \cdot (-\xi_s \lambda^{-1})^{[n_{(-)}(k_s+\pi)-n_s]} R(\lambda) \quad (6.38)$$

with $R(\lambda)$ a polynomial of order $2n_s$ – the claim is proven.

### 6.6 Proof of Eq. (6.5)

Let $\mathcal{L}^{k_y}$ be a path in the constant-$k_y$ interval $[(-\pi,k_y), (\pi,k_y)]$; we choose the path-ordering convention that $k_x$ increases along the path $\mathcal{L}^{k_y}$. We define (i) the time-reversed path $\mathcal{T} \cdot \mathcal{L}^{k_y}$,
which sweeps the same interval with opposite path-ordering (i.e., decreasing \(k_x\)), and (ii) the \(I\)-mapped path \(\mathcal{E} \mathcal{L}^{k_y}\), which sweeps the interval \([(-\pi, -k_y), (\pi, -k_y)]\) with decreasing \(k_x\). In combination, \(\mathcal{E} \mathcal{T} \mathcal{L}^{k_y} = \mathcal{L}^{-k_y}\); this observation leads us to the following identity:

\[
\mathcal{W}^\dagger (\mathcal{L}^{-k_y}) = \mathcal{W}(\mathcal{T} \mathcal{L}^{-k_y}) = B_{\pi,k_y} \mathcal{W}(\mathcal{E} \mathcal{T} \mathcal{L}^{-k_y}) B_{-\pi,k_y}^\dagger
\]

\[
= B_{\pi,k_y} \mathcal{W}(\mathcal{L}^{k_y}) B_{-\pi,k_y}^\dagger.
\] (6.39)

where \(B_k\) are sewing matrices defined in Sec. 6.1.1. The first equality follows from (2.29), the second from (6.18). Since \(B_{\pi,k_y} = B_{-\pi,k_y}\) is unitary, we have shown that \(\mathcal{W}\) along \(\mathcal{L}^{k_y}\) is equivalent to the Hermitian adjoint of \(\mathcal{W}\) along \(\mathcal{L}^{-k_y}\) by a unitary transformation, as advertised.

### 6.7 Wilson Loop of the 2D Time-Reversal Symmetric Insulator

The time-reversal operator is written as \(T = QK\), with \(Q^{-1} = Q^\dagger\) and \(K\) the complex-conjugation operator. On spin-half single-particle states, \(T^2 = -I\), which implies \(Q^T = -Q\). We define a matrix that sews occupied Bloch bands at \(\pm k\) through \(T\): \(V_{k}^{ij} = \langle U^i_k | T | U^j_k \rangle\); \(i, j = 1 \ldots n_{occ}\). \(Q^T = -Q\) implies \(V_{k}^{ij} = -V_{k}^{ji}\). By a similar proof as one presented in Sec. 6.3, one can show that \(V^{-1} = V^\dagger\), which implies \([U^i_k]_a = V_{k}^{ij*} Q_{\alpha \beta} [U^j_k]_{\beta}\).

Applying this relation to a Wilson line between \(-k^{(1)}\) and \(-k^{(2)}\), which are infinitesimally apart:

\[
\mathcal{W}_{-k^{(1)} \rightarrow -k^{(2)}} = \langle U^i_{-k^{(1)}} | U^j_{-k^{(2)}} \rangle
\]

\[
= V_{k(1)}^{il} Q_{\alpha \beta} [U^i_{k(1)}]_{\alpha} V_{k(2)}^{jm*} Q_{\alpha \delta} [U^m_{k(2)}]_{\delta}
\]

\[
\Rightarrow \mathcal{W}_{-k^{(1)} \rightarrow -k^{(2)}} = V_{k(1)}^{il} \mathcal{W}_{k^{(1)} \rightarrow k^{(2)}} V_{k(2)}^{jm*}
\] (6.40)

\[
\Rightarrow \mathcal{W}_{k^{(1)} \rightarrow k^{(2)}} = V_{k(1)}^{il} \mathcal{W}_{k^{(1)} \rightarrow k^{(2)}} V_{k(2)}^{jm*}
\] (6.41)
By employing (2.28), the relation (6.41) is generalizable to finite-length paths, with arbitrary $k^{(1)}, k^{(2)}$. We recall the definitions of $\mathcal{L}^{k_y}$, $\mathcal{T}^{k_y}$, $\mathcal{E} \mathcal{L}^{k_y}$ and $\mathcal{E} \mathcal{T} \mathcal{L}^{k_y}$, as detailed in Sec. 6.6.

\[ W^\dagger (\mathcal{L}^{-k_y}) = W (\mathcal{T} \mathcal{L}^{-k_y}) = V_{\pi,k_y} W (\mathcal{E} \mathcal{T} \mathcal{L}^{-k_y}) V_{-\pi,k_y}^\dagger \]
\[ = V_{\pi,k_y} W (\mathcal{L}^{-k_y}) V_{\pi,k_y}^\dagger. \tag{6.42} \]

The first equality follows from (2.29), the second from (6.18) and the third from $\mathcal{E} \mathcal{T} \mathcal{L}^{k_y} = \mathcal{L}^{-k_y}$. Since $V_{\pi,k_y}$ is unitary, we have shown that $W$ along $\mathcal{L}^{k_y}$ is equivalent to the transpose of $W$ along $\mathcal{L}^{-k_y}$ by a unitary transformation, thus proving (6.8). (6.42) may be written in a familiar form:

\[ W^{-1} (\mathcal{L}^{-k_y}) = \Theta W (\mathcal{L}^{k_y}) \Theta \tag{6.43} \]

with $\Theta = K V_{\pi,k_y}^\dagger$, and satisfying $\Theta^2 = -I$. This implies that each eigenstate of $W_{K_y}$ at $K_y = \{0, \pi\}$ has a degenerate Kramer's partner.

### 6.8 Experimental outlook

We have formulated a $\mathbb{Z}^2$ classification of 1D and 2D insulators with inversion ($\mathcal{I}$) symmetry. Since the Berry phase and inversion eigenvalues of a Bloch band depend on the choice of unit cell, the 1D classification is useful so long as there is a preferred unit cell. In monatomic Bravais lattices, the natural unit cell is centered around the atom. If there are multiple atoms per unit cell, a natural choice of the unit cell may not exist, unless such choice is selected by the presence of an edge. In this sense, the 1D Berry phase reflects boundary physics. An experimentally-relevant example is the boundary charge theorem of Vanderbilt, which relates the charge on an edge to the bulk polarization. [48] Yet another example lies in the entanglement spectrum of 1D insulators, where a spatial entanglement cut mimics an edge. [101,102]

Our results have implications for experiments that directly measure Berry phase through interference. These experiments require coherent transport across the BZ, as has been realized in semiconductor superlattices [103–108] and optical lattices of cold atoms. [109–
Due to the unit cell ambiguity in translationally-invariant systems, the Berry phases are determined only up to a global phase. In 1D, this implies that only differences in Berry phases are physical observables; such differences have been measured by Atala et al. in a cold-atom setting. [82] On the other hand, if a 2D insulator exhibits spectral flow in the Berry phases, such a property is invariant under a global translation of phases. Thus, the relative winding of an $\mathcal{I}$-symmetric insulator is physically observable.
Chapter 7

Berry-Phase Description of
Topological Crystalline Insulators

The first topological crystalline insulator [19] with robust surface modes is protected by the $C_n$ point group (for $n = 4$ and 6), in combination with time-reversal symmetry (TRS). This Chapter presents a case study of these two combined groups, which we refer to collectively as $C_n + T$. Our study is motivated by two issues: (i) In Ref. [19], we learned there exists two distinct gapped phases with $C_n + T$ symmetry, which are distinguished by robust surface modes; we refer to one as the trivial phase and the other a strong topological phase. It is unclear if these two phases are physically distinguishable if we experimentally probe the bulk instead of the surface. (ii) In this letter we highlight the existence of a third topological phase which does not manifest robust surface modes. Does this ‘weak phase’ have any physical consequence? One answer to (i) and (ii) may be found through holonomy, i.e., parallel transport along certain non-contractible loops in the Brillouin zone (BZ) [25, 113, 114]. An electron transported around a loop acquires a Berry-Zak phase [27–29], which has recently been measured by interference in cold-atom experiments [82]. For the purpose of unveiling the bulk topology of all three phases, we find that not all non-contractible loops work. Straight loops are commonly studied in the geometric theory of polarization, due to their relation with Wannier functions [47, 50]; however, these loops cannot identify our weak
phase. Instead, we propose that all three phases are distinguished by parallel transport along \textit{bent} loops, whose shapes are determined by the symmetry group – they are illustrated in Fig. 7.1(a) and (d), for the $C_4 + T$ and $C_6 + T$ groups respectively. Our formulation through holonomy simultaneously reveals a geometric connection with the theory of matrices in $SO(2m)$ – we show that different sectors of ground states have a one-to-one correspondence with distinct classes of rotations.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7_1.png}
\caption{(a) (resp. (d)) illustrates certain bent loops in the 3D Brillouin zone of a simple tetragonal (resp. hexagonal) lattice. (b) and (c): Berry-phase spectrum of trivial and strong phases respectively, for the model of (7.3). (e) and (f): Berry-phase spectrum of trivial and strong phases, for a $C_6 + T$ model described in Sec. 7.3.}
\end{figure}

After a brief review of the relevant symmetries in a tight-binding context (Sec. 7.1), we present our main results in Sec. 7.2. The remaining Sections are more technical: in Sec. 7.3, we provide the details of a $C_6 + T$ model that has been employed in Sec. 7.2. In Sec. 7.4, we review general properties of the Wilson loop. In Sec. 7.5, we derive certain properties of the bent Wilson loop $W[l_n(k_z)]$, as applied to the $C_n + T$ insulator; these properties apply for any $k_z$ in the Brillouin zone. In Sec. 7.6, we focus on $W[l_n(\bar{k}_z)]$ in the high-symmetry planes defined by $\bar{k}_z = 0$ and $\pi$. Specifically, we develop a geometric interpretation of $W[l_n(\bar{k}_z)]$ as a special type of proper rotation, and derive the structure of its spectrum. In Sec. 7.7, we show an alternative formulation of the topological invariant $\Gamma_n$, to make contact with previous work in Ref. [19]. In Sec. 7.8, we describe how the choice
of the spatial origin affects the Berry-Zak phases, and describe a translational-invariant formulation of the $C_n + T$ topological invariants. We conclude with a brief outlook in Sec. 7.9.

7.1 Review of symmetries in the tight-binding Hamiltonian

Here, we supplement Sec. 1.2 with a few examples that are relevant to this chapter. Let us consider a tetragonal lattice with a two-atom unit cell – the lattice is composed of two interpenetrating cubic sublattices, which are correspondingly colored red and blue in Fig. 3.6(a). Our tight-binding basis comprises $(p_x, p_y)$ orbitals on each sublattice, which we label by $\alpha = 1$ (resp. 2) for $p_x + ip_y$ (resp. $p_x - ip_y$) orbitals on the blue sublattice, and $\alpha = 3$ (resp. 4) for $p_x - ip_y$ (resp. $p_x + ip_y$) orbitals on the red sublattice. Suppose the spatial origin lies on an atomic site in the blue sublattice, e.g., the corner of the cube in Fig. 3.6(a).

With this choice of origin, the spatial embeddings are $r_1 = r_2 = 0$, and $r_3 = r_4 = \Delta \hat{z}$ corresponds to the vertical offset between the two sublattices.

![Figure 7.2: (a) Tetragonal lattice. Each blue sphere corresponds to an atom in one cubic sublattice; red spheres belong to a second cubic sublattice. The unit cell is encircled by a dashed rectangle, and one choice for the spatial origin is the blue atomic site in this rectangle. (b) Top-down view of tetragonal lattice.](image)

Let us define $U_{2\pi/n}$ ($R_{2\pi/n}$) is defined as the matrix representation of a $C_n$-rotation in the basis of Löwdin orbitals (in $\mathbb{R}^d$, where $d$ is the dimension of the Brillouin zone). Equivalently, the crystal momenta $\mathbf{k}$ and $R_{2\pi/n} \mathbf{k}$ are related by: $R_{2\pi/n}(k_x, k_y, k_z) = (k_x \cos 2\pi/n - k_y \sin 2\pi/n, k_y \cos 2\pi/n + k_x \sin 2\pi/n, k_z)$. The Bloch Hamiltonian of a $C_n + T$ insulator
has the $C_n$ symmetry [60]:

$$U_{2\pi/n} H(k) [U_{2\pi/n}]^{-1} = H(R_{2\pi/n} k), \quad (7.1)$$

and the time-reversal symmetry

$$TH(k) T^{-1} = H(-k). \quad (7.2)$$

Without spin-orbit coupling, our wavefunctions transform with integral angular momentum. Hence, under $C_n$ rotation, $[U_{2\pi/n}]^n = I$; under time-reversal, $T^2 = I$.

### 7.2 $C_n + T$ insulators

It is known from Ref. [19] that the $C_n + T$ insulator is characterized by two $\mathbb{Z}_2$ indices $\{ \Gamma_n(\bar{k}_z) \}$, for $\bar{k}_z \in \{0, \pi\}$; $\Gamma_n(0) \in \{+1, -1\}$ describes the Bloch wavefunctions in the plane $k_z = 0$. In analogy with the spin-orbit-coupled $Z_2$ insulator, $\{ \Gamma_n(0), \Gamma_n(\pi) \}$ shall be referred to as weak indices [13, 16, 19]. $\Gamma_n(0) = \Gamma_n(\pi) = 1$ ($-1$) corresponds to the trivial (weak) phase, and $\Gamma_n(0) = -\Gamma_n(\pi)$ describes a strong phase. The product $\Gamma_n(0) \Gamma_n(\pi)$ is a strong index that determines the absence or presence of robust surface modes on the 001 surface; we take $\hat{z}$ to lie along the principal $C_n$ axis. We give these weak indices a physically transparent interpretation from the perspective of holonomy. For illustration, we consider a $C_4 + T$ model on the tetragonal lattice that is described in Sec. 7.1 and illustrated in Fig. 7.2(a). Our tight-binding basis comprises $(p_x, p_y)$ orbitals on each sublattice; each pair transforms in the two-dimensional irreducible representation (irrep) of $C_4 + T$. By this, we mean that the $p_x \pm ip_y$ orbitals are eigenstates of four-fold rotation, while time-reversal maps $p_x + ip_y \rightarrow p_x - ip_y$. In short, we call such irreps doublets, and all other irreps are singlets. The Bloch Hamiltonian is

$$H(k) = \left[ -1 + 8 f_1(k) \right] \Gamma_{03} + \left[ 2 f_2(k) + \delta f_6(k) \right] \Gamma_{11} + \alpha f_4(k) \Gamma_{01} + \beta f_5(k) \Gamma_{32} + 2 f_6(k) \Gamma_{12}, \quad (7.3)$$

where $f_1 = 3 - \cos(k_x) - \cos(k_y) - \cos(n_z k_z)$, $f_2 = 2 - \cos(k_x) - \cos(k_y)$, $f_3 = \cos(k_z)$, $f_4 = \cos(k_y) - \cos(k_x)$, $f_5 = \sin(k_x) \sin(k_y)$ and $f_6 = \sin(n_z k_z)$. In $\Gamma_{ab} = \sigma_a \otimes \tau_b$, $\sigma_i$ and $\tau_i$...
are Pauli matrices for \( i \in \{1, 2, 3\} \), while \( \sigma_0 \) and \( \tau_0 \) are identities in each 2D subspace. \( |\sigma_3 = \pm 1, \tau_3 = +1\rangle \) label \( \{p_x \pm ip_y\} \) orbitals on one sublattice, and \( |\sigma_3 = \pm 1, \tau_3 = -1\rangle \) label \( \{p_x \mp ip_y\} \) orbitals on the other. This Hamiltonian is four-fold symmetric: \( \Gamma_{33} H(k_x, k_y, k_z) \Gamma_{33} = H(-k_y, k_x, k_z) \), and time-reversal symmetric: \( \Gamma_{10} H(k) \Gamma_{10} = H(-k) \). The ground state of (7.3) comprises its two lowest-lying bands. The phase diagram of this model is plotted in Fig. 7.3(a) for different parametrizations of (7.3).

Figure 7.3: (a) Phase diagram of \( C_4 + T \) model (7.3), as parametrized by \( \alpha \) and \( \beta \); we fix \( n_z = 1 \) and \( \delta = 0 \). Blue (uncolored) regions correspond to gapped (gapless Weyl) phases [60]. The weak indices in each gapped phase are indicated by \( \{\Gamma_4(0), \Gamma_4(\pi)\} \). The blue square in the center is approximately bound by \( |\alpha| < 2 \) and \( |\beta| < 2 \). The 001-surface spectrum is plotted for two representative points on the phase diagram: (b) for \( \alpha = \beta = 1 \), and (c) for \( \alpha = \beta = 4 \). \( \bar{\Gamma}, M \) and \( \bar{X} \) are high-symmetry momenta defined in Fig. 3.6(a).

To probe the bulk topology, we perform parallel transport along a bent loop that connects two \( C_4 \)-invariant points; \( C_n \)-invariant points refer to momenta which are invariant under an \( n \)-fold rotation, up to a reciprocal lattice vector. We define \( l_4(0) \) as the loop connecting \( M - \Gamma - M \) in the \( k_z = 0 \) plane, and \( l_4(\pi) \) connects \( A - Z - A \) in the \( k_z = \pi \) plane. They are respectively depicted by red and brown lines in Fig. 7.1(a). As we review in Sec. 2, the matrix representation of holonomy is known as the Wilson loop \( W[l] \); \( l \) denotes a loop and \( W \) is a matrix with dimension equal to the number \( (n_{occ}) \) of occupied bands. The gauge-invariant spectrum of \( W[l] \) is also known as the Berry-Zak phase factors (\( \{\exp(i\vartheta)\} \)) [28, 29, 33]. Let us show that the spectrum of \( W[l_4(\bar{k}_z)] \) encodes the weak index \( \Gamma_4(\bar{k}_z) \). If we define \( d_4 \) is the number of \(-1\) eigenvalues in the spectrum of \( W[l_4(\bar{k}_z)] \), then the weak indices \( \{\Gamma_4(0), \Gamma_4(\pi)\} \) are related to \( \{d_4(0), d_4(\pi)\} \) by

\[
\Gamma_n(\bar{k}_z) = i^{d_n(\bar{k}_z)} \in \{1, -1\}; \quad \bar{k}_z \in \{0, \pi\}
\]

for \( n = 4 \); as we will shortly clarify, \( d_4 \) is necessarily even. This weak index is equivalent
to an alternative formulation in Ref. [19], where it is expressed as an invariant involving the Pfaffian of a matrix; cf. Sec. 7.7. We provide a geometrical interpretation of (7.4): the parity of $d_4(\vec{k}_z)/2$ specifies one of two classes of a special rotation, which is in one-to-one correspondence with two sectors of ground states in the $k_z = \bar{k}_z$ plane. The following discussion briefly clarifies the nature of this rotation; further details may be found in Sec. 7.6. Due to two-fold rotational and TRS, we can choose a basis in which $W[l_4(\vec{k}_z)] \in SO(n_{\text{occ}})$, i.e., they are proper rotations in $\mathbb{R}^{n_{\text{occ}}}$. Since the bands derive from doublet orbitals, $n_{\text{occ}}$ is even. A rotation $R$ in $n_{\text{occ}} = 2m$ dimensions is described by $m$ invariant planes, and an angle of rotation in each plane. If all $m$ angles equal to $\theta$, such a rotation is called equiangular – there is an invariant plane through any arbitrary vector of space and all vectors are rotated by the same angle $\theta$ [115]. In an appropriate basis, $W[l_4(\vec{k}_z)]$ is a product of two equiangular rotations, each of angle $\pi/2$ – the net effect is that a vector may be maximally rotated by angle $\pi$. The set of vectors which are rotated by $\pi$ is defined as the maximally-rotated subspace, and we interpret $d_4(\vec{k}_z)$ in (7.4) as the dimension of this subspace. These vectors always come in pairs, since each eigenvalue of an even-dimensional rotation has a complex-conjugate partner [115]. There are then two classes of $W$ distinguished by the parity of $d_4(\vec{k}_z)/2$; in the nontrivial (trivial) class an odd (even) number of pairs are maximally rotated. The simplest example for $n_{\text{occ}} = 2$ is the equiangular rotation $R_\pm = e^{\pm i \sigma_2 \pi/2}$. $W$ is either the trivial identity: $R_+ R_- = I$, or it rotates any vector by $\pi$: $R_+ R_- = -I$. Now we demonstrate how to realize both classes of $W$ in the model of (7.3). Let us consider a family of loops $\{l_4(k_z)\}$ in planes of constant $k_z$, such that $l_4(0)$ is the red line in Fig. 7.1(a), and all other loops project to $l_4(0)$ in $\hat{z}$. In the trivial phase (parametrized by $\alpha = \beta = 1$), we find $W[l_4(0)] = W[l_4(\pi)] = I$, or equivalently $\Gamma_4(0) = \Gamma_4(\pi) = +1$. The eigenvalues of $W[l_4(k_z)]$ interpolate between $\{1, 1\}$ (at $k_z = 0$) to $\{1, 1\}$ (at $k_z = \pi$), as illustrated in Fig. 7.1(b). The absence of surface modes on the line $\bar{M} - \bar{\Gamma} - \bar{X}$ is demonstrated in Fig. 7.3(b). In comparison, the strong phase ($\alpha = \beta = 4$) is characterized by $W[l_4(0)] = -W[l_4(\pi)] = -I$, or $\Gamma_4(0) = -\Gamma_4(\pi) = -1$; its surface modes are illustrated in Fig. 7.3(c). As $k_z$ is varied from 0 to $\pi$ in Fig. 7.1(c), the Berry phases $\{\vartheta(k_z)\}$ interpolate across the maximal range
\([-\pi, \pi]\) – we call this property spectral flow. In comparison, the weak phase is identified by \(W[l_4(0)] = W[l_4(\pi)] = -I\), which clearly does not exhibit spectral flow. Finally, we point out that the definition of the weak index through (7.4) is only meaningful if we specify the spatial origin; it is possible to formulate the weak index in a translational-invariant manner, as we elaborate in Sec. 7.8.

Figure 7.4: Characterization of the \(C_6 + T\) insulator. (a) (resp. (b)) is the 001-surface spectrum of a trivial (resp. strong) insulator. \(\Gamma, K\) and \(\tilde{K}_2\) are \(C_3\)-invariant momenta defined in Fig. 3.6(b). (c), (d) and (e) respectively illustrate the Berry phases of trivial, weak and topological phases.

The story of the \(C_6 + T\) insulator proceeds analogously. We provide a model whose details are reported in Sec. 7.3; the trivial and strong phases of this model are distinguished by surface modes, as illustrated in Fig. 7.4(a) and (b). The bulk topology is unveiled by the following bent loops, which are illustrated in Fig. 7.1(d): we define \(l_6(0)\) as the loop \(K - \Gamma - K\) (red), and \(l_6(k_z)\) as the \(\hat{z}\)-projection of \(l_6(0)\) in the plane of constant \(k_z\). In principle, we may consider a second family of \(C_6\) Wilson loop which connects \(K_2 - \Gamma - K_2\), where \(K_2\) is the second \(C_3\)-invariant point on the vertex of the hexagonal BZ; due to \(C_6\) symmetry, this loop is related to (7.8) by a unitary transformation, and thus contains no new information. For \(\tilde{k}_z \in \{0, \pi\}\), a basis may be found where \(W[l_6(\tilde{k}_z)]\) is a product of two equiangular rotations, each of angle \(\pi/3\) – a vector may be maximally rotated by an angle \(2\pi/3\), as we show in Sec. 7.6. (7.4) similarly applies for \(n = 6\), if we define \(d_6\) as the dimension of the maximally-rotated subspace. Equivalently, \(d_6/2\) is the number of \(\exp(i2\pi/3)\)-eigenvalues in the spectrum of \(W[l_6(\tilde{k}_z)]\). Like \(\Gamma_4, \Gamma_6\) is also equivalent to a Pfaffian invariant, though the
proposed formula in Ref. [19] requires a clarification; cf. Sec. 7.7. In the strong phase, the Berry phases interpolate across the maximal range \([-2\pi/3, 2\pi/3]\); compare Fig. 7.1(e) with Fig. 7.1(f).

Beyond these two models, we would like to generalize our results to insulators with any number of occupied doublet bands. For \(n \in \{4, 6\}\), the spectrum of \(W[l_n(k_z)]\) falls into two classes which are labelled by the weak index \(\Gamma_n(k_z) \in \{\pm 1\}\); the structure of the two classes is laid out in Tab. 7.1. In the strong phase, \(\Gamma_n(0) = -\Gamma_n(\pi)\) is a sufficient condition for spectral flow: the Berry phases \(\{\vartheta(k_z)\}\) robustly interpolate across the full range \([-4\pi/n, 4\pi/n]\), in the interval \(k_z \in [0, \pi]\). The converse is also true for the trivial and weak phases: \(\Gamma_n(0) = \Gamma_n(\pi)\) implies the lack of spectral flow. Though a proof can be written, we prefer to make a pictorial argument through Fig. 7.4(c) to (e), where we compare trivial, weak and strong phases in a \(C_6 + T\) model with four occupied bands.

Crucial to this argument is that \(\{\vartheta(k_z)\}\) satisfy certain symmetry constraints: (i) for any \(k_z \in [0, \pi]\), the spectrum of \(W\) only comprises complex-conjugate pairs \(\{\exp(i\vartheta), \exp(-i\vartheta)\}\), as proven in Sec. 7.5, and (ii) all \(W\)-eigenvalues are doubly-degenerate at \(k_z = 0\) and \(\pi\) (cf. Tab. 7.1).

<table>
<thead>
<tr>
<th>(n_{occ})</th>
<th>(\Gamma_n)</th>
<th>Spectrum of (W[l_n(k_z)])</th>
</tr>
</thead>
<tbody>
<tr>
<td>4m</td>
<td>1</td>
<td>({\lambda_1}_4, {\lambda_2}_4, \ldots, {\lambda_m}_4)</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>(e^{i4\pi/n}, e^{-i4\pi/n}, 1, 1, {\lambda_1}<em>4, \ldots, {\lambda</em>{m-1}}_4)</td>
</tr>
<tr>
<td>4m + 2</td>
<td>1</td>
<td>1, 1, {\lambda_1}_4, \ldots, {\lambda_m}_4</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>(e^{i4\pi/n}, e^{-i4\pi/n}, {\lambda_1}_4, \ldots, {\lambda_m}_4)</td>
</tr>
</tbody>
</table>

Table 7.1: Spectrum of the bent Wilson loop. We consider two cases: (i) the number of occupied bands \(n_{occ}\) is \(4m\), for non-negative integer \(m\), and (ii) \(n_{occ} = 4m + 2\). In either case, the spectrum has two possible structures, as labelled by \(\Gamma_n \in \{+1, -1\}\). \(\{\lambda_1\}_4\) denotes a doubly-degenerate eigenvalue and its complex conjugate: \(\{\lambda_1, \lambda_1, \lambda_1^*, \lambda_1^*\}\). This table is derived in Sec. 7.6.

Finally, we point out an alternative characterization of the \(C_n + T\) insulator by Berry phases, which was described in Ref. [50] for a different choice of loop. Their characterization is useful to identify the strong index: the product \(\Gamma_n(0)\Gamma_n(\pi)\), but cannot individually distinguish the weak indices: \(\Gamma_n(0)\) and \(\Gamma_n(\pi)\).
7.3 Model of $C_6 + T$ insulator

We model a $C_6 + T$ insulator on a hexagonal Bravais lattice; this model is a generalization of the $C_4 + T$ model proposed in Ref. [19]. The unit cell comprises two inequivalent atoms $A$ and $B$ along the $c$-axis, and each atom belongs to a triangular lattice – the entire crystal may be thought of as stacked bilayers of triangular lattices. The orbitals on each atom transform in the \{p_x, p_y\} representation. Our basis is spanned by the Pauli matrices $\tau_i$ and $\sigma_i$: the A-sublattice (B-sublattice) corresponds to $\tau_3 = +1$ ($-1$), and the $p_x$ ($p_y$) orbital corresponds to $\sigma_3 = +1$ ($-1$). The Hamiltonian may be written as

$$H(k) = \begin{pmatrix} h_{AA}(k) & h_{AB}(k) \\ h_{AB}(k)^\dagger & h_{BB}(k) \end{pmatrix}, \quad (7.5)$$

such that $h_{aa}$ acts within the sublattice $a \in \{A, B\}$. We consider sigma-type hopping within each sublattice: nearest-neighbor (next-nearest-neighbor) hoppings are parametrized by $t_1^a$ ($t_2^a$).

$$h_{aa}(k) = t_1^a \begin{pmatrix} 2 \cos k_1 + \frac{1}{2} \cos k_2 + \frac{1}{2} \cos (k_1 - k_2) & \frac{\sqrt{3}}{2} \cos k_2 - \frac{\sqrt{3}}{2} \cos (k_1 - k_2) \\ \frac{\sqrt{3}}{2} \cos k_2 - \frac{\sqrt{3}}{2} \cos (k_1 - k_2) & \frac{3}{2} \cos k_2 + \frac{3}{2} \cos (k_1 - k_2) \end{pmatrix} + t_2^a \times$$

$$\begin{pmatrix} \frac{3}{2} \cos (k_1 + k_2) + \frac{3}{2} \cos (2k_1 - k_2) & \frac{\sqrt{3}}{2} \cos (k_1 + k_2) - \frac{\sqrt{3}}{2} \cos (2k_1 - k_2) \\ \frac{\sqrt{3}}{2} \cos (k_1 + k_2) - \frac{\sqrt{3}}{2} \cos (2k_1 - k_2) & 2 \cos (2k_2 - k_1) + \frac{1}{2} \cos (k_1 + k_2) + \frac{1}{2} \cos (2k_1 - k_2) \end{pmatrix}$$

Here, we have chosen the non-orthogonal coordinates \{k_1, k_2, k_z\}, defined by $k = (k_1 b_1 + k_2 b_2 + k_z b_3) / 2\pi$; $k_1, k_2, k_z \in [0, 2\pi)$; the reciprocal lattice vectors are $b_1 = b/(\sqrt{3}, -1, 0)$, $b_2 = b (0, 1, 0)$ and $b_3 = 2\pi/c (0, 0, 1)$ for some parameters $b$ and $c$.

We include inter-sublattice orbital-independent hoppings: nearest-neighbor (next-nearest-neighbor) hoppings within a bilayer are parametrized by $t_1'$ ($t_2'$); nearest-neighbor hoppings
between bilayers are parametrized by $t'_{z}$.

$$h_{AB}(k) = (t'_1 + 2t'_2 (\cos k_1 + \cos k_2 + \cos (k_1 - k_2)) + t'_z e^{ik_z}) I. \quad (7.6)$$

This Hamiltonian has the time-reversal symmetry: $H(k)^* = H(-k)$, and six-fold symmetry: $U_{\pi/3} H(k) U_{-\pi/3}^{-1} = H(R_{\pi/3} k)$, for $U_{\pi/3} = \exp[-i\sigma_2\pi/3]$; $k$ and $R_{\pi/3} k$ are two momenta related by a six-fold rotation.

We choose the parameters $t^A_1 = -t^B_1 = 1$, $t^A_2 = -t^B_2 = 0.5$, $t'_1 = 2.5$, $t'_2 = 0.5$. For $t'_z = 0.5$ (resp. 2), the phase is trivial (resp. strong) and its Berry-phase spectrum is illustrated in Fig. 7.1(e) (resp. (f)). The surface modes are respectively illustrated in Fig. 7.4(a) and (b).

### 7.4 Some useful properties and notations for Wilson loops

In the $n_{occ}$-dimensional basis of occupied bands, the generic Wilson loop $W \in U(n_{occ})$. Following standard convention, we define $U(n_{occ})$ ($SU(n_{occ})$) as the group of (special) unitary matrices in $n_{occ}$ dimensions; similarly, $O(n_{occ})$ ($SO(n_{occ})$) as the group of (special) orthogonal matrices in $n_{occ}$ dimensions. Since we focus on bands which derive from doublet irreps of $C_n + T$, $n_{occ}$ is even. In the proofs below, notation is greatly simplified if we assume that all orbitals within a unit cell lie on the same atom; the generalization to arbitrary spatial embeddings is straightforward, and we refer the interested reader to Ref. [60].

We are interested in $W[l_n(k_z)]$, where $l_n(k_z)$ denotes a bent loop in a plane of constant $k_z$; these loops are defined in the main text. It is convenient to express each of these loops as a product of two Wilson lines. In the case of $C_4 + T$,

$$W[l_4(k_z)] = W_{b \rightarrow a}(k_z) W_{a \rightarrow b}(k_z) \in U(n_{occ}), \quad (7.7)$$

where $W_{a \rightarrow b}$ is an in-plane Wilson line that connects momenta $a = (-\pi, \pi, k_z)$ to $b = (0, 0, k_z)$ along a diagonal in the upper-left quadrant (red line in Fig. 7.5(a)); $W_{b \rightarrow a}$ is an in-plane Wilson line that connects $b = (0, 0, k_z)$ to $\bar{a} = (\pi, \pi, k_z)$ along a diagonal in the upper-right quadrant (blue line in Fig. 7.5(a)); the momenta $a$ and $\bar{a}$ are connected by a
reciprocal lattice vector. Analogously, we express
\[ W[l_6(k_z)] = W_{d \rightarrow c}(k_z) W_{c \rightarrow d}(k_z) \in U(n_{occ}), \]  
(7.8)
where we define the \( C_3 \)-invariant momenta: \( c = (-2\pi/3, 2\pi/\sqrt{3}, k_z) \), \( d = (0, 0, k_z) \) and \( \bar{c} = (4\pi/3, 0, k_z) \); \( c \) and \( \bar{c} \) are connected by a reciprocal lattice vector. \( W_{c \rightarrow d} \) (\( W_{d \rightarrow c} \)) is illustrated in red (blue) in Fig. 7.5(b). Certain properties \( W[l_n(k_z)] \) for \( k_z \in \{0, \pi\} \) are not shared by \( W[l_n(k_z)] \) for general \( k_z \). For example, the geometric interpretation of \( W \) as a special rotation only applies for \( k_z \in \{0, \pi\} \). The reader is thus advised to distinguish between \( k_z \) and \( \bar{k}_z \) in various contexts.

Figure 7.5: (a) A constant-\( k_z \) plane in the 3D Brillouin zone of a tetragonal lattice. \( a, \bar{a} \) and \( b \) are \( C_4 \)-invariant momenta, with \( a \) and \( \bar{a} \) identified by a reciprocal lattice vector. (b) A constant-\( k_z \) plane in the 3D Brillouin zone of a hexagonal lattice. \( c, \bar{c} \) and \( d \) are \( C_3 \)-invariant momenta, with \( c \) and \( \bar{c} \) identified by a reciprocal lattice vector.

7.5 Analytic properties of \( W[l_n(k_z)] \in U(n_{occ}) \) for general \( k_z \)

7.5.1 Bounds on the eigenvalues of \( W[l_6(k_z)] \in U(n_{occ}) \) for general \( k_z \), as applied to the \( C_6 + T \) insulator

Consider the eigenvalues \( \{ \exp(i\vartheta_j(k_z)) \} \) of a family of loops \( W[l_6(k_z)] \in U(n_{occ}) \), which are defined in (7.8). \( j \in \{1, 2, \ldots, n_{occ}\} \) labels the eigenvalue. We define \( \vartheta_j \) as lying in the principal branch, i.e., \( -\pi < \vartheta_j \leq \pi \). In this section we derive the following result: within this family of loops, \( |\vartheta_j(k_z)| \leq 2\pi/3 \) for all \( j \) and \( k_z \).

Proof: Following our definitions of \( c, \bar{c}, \) and \( d \) in Sec.7.4, the occupied bands \( \{u_{i,k}\} \) along the lines \( c \searrow d \) and \( d \rightarrow \bar{c} \) are related by \( C_3 \) symmetry, as illustrated in Fig. 7.5(b). This
motivates us to consider the matrix representation of $C_3$ in the basis of occupied doublet bands:

$$[B_{2\pi/3}(k)]_{ij} = \langle u_i, R_{2\pi/3} k | U_{2\pi/3} | u_j, k \rangle,$$

where

$$R_{2\pi/3} = \begin{pmatrix} k_x & k_y & k_z \\ k_y \cos \frac{2\pi}{3} - k_y \sin \frac{2\pi}{3} & k_y \cos \frac{2\pi}{3} + k_x \sin \frac{2\pi}{3} & k_x \sin \frac{2\pi}{3} \\ k_x & k_y & k_z \end{pmatrix},$$

and $U_{2\pi/3}$ represents a rotation of $2\pi/3$ in the basis of Löwdin orbitals. We define $k_i$ as $C_3$-invariant momenta for which $R_{2\pi/3}(k_i) = k_i$ up to reciprocal lattice vectors. The bands at $k_i$ form doublets with $C_3$-eigenvalues $\exp(\pm i\frac{2\pi}{3})$, thus a general form for $B(k_i)$ is

$$B_{2\pi/3}(k_i) = F(k_i) e^{iR\frac{2\pi}{3}} F(k_i)\dagger,$$

where $F(k_i) \in U(n_{occ})$, $R = \bigoplus_{j=1}^{m} \sigma_3$ is a block-diagonal matrix and $\sigma_3$ is a Pauli matrix. Due to the $C_3$ symmetry relating bands along $c \uparrow d$ and $d \rightarrow \bar{c}$, we deduce from (7.8) that

$$W[l_6(k_z)] = B_{2\pi/3}(c)\dagger W_{c \uparrow d}(k_z)\dagger B_{2\pi/3}(d) W_{c \uparrow d}(k_z).$$

Here, we have related $W_{d \rightarrow c}$ to $W_{c \uparrow d}^\dagger$, where the Hermitian conjugation arises because rotating $c \uparrow d$ by angle $2\pi/3$ produces $d \rightarrow \bar{c}$ with the reverse orientation. For more details of the algebraic steps leading to (7.12), the interested reader may refer to an analogous calculation in Ref. [33]. Let us then define

$$\tilde{R}(k_z) = F(c)\dagger W_{c \uparrow d}(k_z)\dagger F(d) R F(d)\dagger W_{c \uparrow d}(k_z) F(c).$$

Since $F(d)\dagger W_{c \uparrow d}(k_z) F(c)$ is a product of unitary matrices, it is itself unitary. We then find that $W[l_6(k_z)]$ is equivalent to $e^{-iR\frac{2\pi}{3}} e^{i\tilde{R}(k_z)\frac{2\pi}{3}}$, up to a unitary transformation. We denote this unitary equivalence by the symbol $\sim$:

$$W[l_6(k_z)] \sim e^{-iR\frac{2\pi}{3}} e^{i\tilde{R}(k_z)\frac{2\pi}{3}} = e^{iR\frac{\pi}{3}} e^{-i\tilde{R}(k_z)\frac{\pi}{3}};$$

(7.14)
the last equality follows from $R^2 = \tilde{R}^2 = I$. We employ a theorem proven in Ref. [116–118], which sets a bound on the eigenvalues of a product of two unitary matrices $U_1$ and $U_2$, given the eigenvalues of each matrix. Let us denote the largest argument of the eigenvalue of a matrix $M$ as $\maxarg[M]$. The theorem states: if $\maxarg[U_1] + \maxarg[U_2] \leq \pi$, then $\maxarg[U_1U_2] \leq \maxarg[U_1] + \maxarg[U_2]$. In our application,

$$\maxarg[e^{iR\pi/3}] = \maxarg[e^{-i\tilde{R}(k_z)\pi/3}] = \pi/3$$

$$\Rightarrow \maxarg[\mathcal{W}[l_6(k_z)]] \leq 2\pi/3. \quad (7.15)$$

We point out that an analogous argument for $\mathcal{W}[l_4(k_z)] \in U(n_{occ})$, as applied to the $C_4 + T$ insulator, leads to the trivial bound $\maxarg[\mathcal{W}[l_4(k_z)]] \leq \pi$.

### 7.5.2 Proof that $\mathcal{W}[l_n(k_z)] \in U(n_{occ})$ has unit determinant, for general $k_z$

In the $C_0 + T$ case, it follows directly from (7.12) and that $B_{2\pi/3}(k_i)$ also has unit determinant, as made apparent in the form (7.11).

The $C_4 + T$ case proceeds in analogous fashion. We define the matrix representation of $C_4$ in the basis of occupied doublet bands:

$$[B_{\pi/2}(k)]_{ij} = \langle u_i, R_{\pi/2}k | U_{\pi/2} | u_j, k \rangle; \quad (7.16)$$

$R_{\pi/2}(k_x, k_y, k_z) = (-k_y, k_x, k_z)$; $U_{\pi/2}$ represents a rotation of $\pi/2$ in the basis of Löwdin orbitals. We define $k_i$ as $C_4$-invariant momenta for which $R_{\pi/2}(k_i) = k_i$ up to reciprocal lattice vectors. The bands at $k_i$ form doublets with $C_4$-eigenvalues $\pm i$, thus a general form for $B(k_i)$ is

$$B_{\pi/2}(k_i) = F(k_i) e^{i\mathcal{R}\pi/2} F(k_i)^\dagger; \quad F(k_i) \in U(n_{occ}), \quad (7.17)$$

where, again, $\mathcal{R} = \bigoplus_{j=1}^m \sigma_3$. Following our definitions of $a, a, \bar{a}$, and $b$ in Sec.7.4, the occupied bands $\{u_i,k\}$ along the lines $b \nearrow \bar{a}$ and $a \swarrow b$ are related by $C_4$ symmetry. Thus from (7.7) [33],

$$\mathcal{W}[l_4(k_z)] = B_{\pi/2}(a)^\dagger \mathcal{W}_a \phi(k_z)^\dagger B_{\pi/2}(b) \mathcal{W}_a \phi(k_z). \quad (7.18)$$
It is clear from (7.17) that $B_{\pi/2}(k_i)$ has unit determinant, thus taking the determinant of (7.18) produces the desired result.

7.6 Analytic properties of $W[l_n(\bar{k}_z)] \in SO(n_{occ})$ for specific $\bar{k}_z \in \{0, \pi\}$

This appendix describes the bent Wilson loop $W[l_n(\bar{k}_z)]$ in the high-symmetry planes $\bar{k}_z = 0$ and $\pi$. In Sec.7.6.1 and 7.6.2, we show that in an appropriate basis, $W$ is a special type of proper rotation. We describe the nature of this rotation in Sec.7.6.3; here the discussion aims to develop a geometric intuition and is less technical. As a prelude to deriving the spectrum of $W$ in Sec.7.6.5, we summarize in Sec.7.6.4 certain useful ideas in the representation theory of Lie groups.

7.6.1 A real, periodic basis is found where $W[l_n(\bar{k}_z)] \in SO(n_{occ})$

**Proof**: Let us define $C_2 T$ as the product of a two-fold rotation and a time reversal. In the planes of constant $\bar{k}_z \in \{0, \pi\}$, $C_2 T$ maps a momentum to itself. We define the matrix representation of $C_2 T$ in the basis of occupied bands as: $[V_{\pi}(k)]_{ij} = \langle u_i, k | U_{\pi} T | u_j, k \rangle$, with $T = Q\tilde{K}$ an antiunitary operator. Applying $(U_{\pi})^2 = I$, $[U_{\pi}, T] = 0$, and $Q = Q^t$, we find that $U_{\pi} Q$ (and hence $V_{\pi}$ also) is symmetric. A unitary, symmetric matrix can be written as $V_{\pi} = F D F^t$, where $F$ is a real orthogonal matrix and $D$ is a diagonal matrix with unimodular eigenvalues $\{\exp(i\phi_j)\}$. Under $U(n_{occ})$ gauge transformations, $|u_{i,k}\rangle \rightarrow \sum_j |u_{j,k}\rangle J(k)_{ji}$, $V_{\pi}(k) \rightarrow J(k)^t V_{\pi}(k) J(k)^*$.

Choosing $J(k) = F(k)$, we diagonalize $V_{\pi}$: $U_{\pi} T |u_{j,k}\rangle = e^{i\phi_{j,k}} |u_{j,k}\rangle$. Note that the matrix representation of an antiunitary operator cannot generically be diagonalized; crucial to this diagonalization is that $V_{\pi}$ is symmetric, thus its eigenvectors can be chosen to be real. By a second transformation $|u_{j,k}\rangle \rightarrow e^{i(\phi_{j,k} - \pi)/2} |u_{j,k}\rangle$, we arrive at:

$$U_{\pi} T |u_{j,k}\rangle = -|u_{j,k}\rangle$$

(7.19)
for all $j \in \{1, 2, \ldots, n_{\text{occ}}\}$. Equivalently, this basis choice results in $V_{\pi}(k) = -I$, i.e., for each band $j$ and momentum $k$, $u_{j,k}$ transforms in the real vector representation of $C_2^T$, e.g., a $p_x$ orbital. We thus call (7.19) a real gauge. Now we show that $W[l_n(\bar{k}_z)] \in SO(n_{\text{occ}})$ in a certain basis. The basis is defined by choosing a set of occupied Bloch wavefunctions \{\$u_{i,k}\$\}, for each momentum along the loop $l_n(\bar{k}_z)$. Let us define $k^{(0)}$ and $k^{(0)} + G$ as the base and end points of the loop, for some reciprocal lattice vector $G$.

**Definition:** In the real, periodic basis, (i) (7.19) is satisfied for all $k$ in the loop $l_n(\bar{k}_z)$, and (ii) the basis is periodic in the sense of $\langle u_{i,k^{(0)} + G} \rangle = \langle u_{i,k^{(0)}} \rangle$ for all $i \in \{1, 2, \ldots, n_{\text{occ}}\}$.

The second condition is implicit in the definition of the Wilson loop, and a generalization exists for nontrivial spatial embeddings of the orbitals [60]. One may verify that (i) and (ii) can be imposed consistently, though the resulting basis is not necessarily differentiable in $k$; as explained in Sec. 7.4, differentiability is not required in the discrete formulation of $W$.

It should be noticed that (i) and (ii) does not fully specify the basis. While maintaining the reality condition (i), we are free to make orthogonal gauge transformations: $\langle u_{i,k} \rangle \rightarrow \sum_j \langle u_{j,k} \rangle U(k)_{ji}$ for $U(k) \in O(n_{\text{occ}})$. The periodic condition (ii) is also maintained so long as $U(k^{(0)}) = U(k^{(0)} + G)$.

It follows from (i) that the overlap matrix $S(k_1, k_2)$, as defined in (2.27), is real for any $k_1$ and $k_2$ on the loop. Since $W$ is expressible as a product of overlap matrices (as shown in (2.28)), $W = W^* \in O(n_{\text{occ}})$. Since $W$ also has unit determinant, as proven in Sec. 7.5.2, $W \in SO(n_{\text{occ}})$. By the same argument, one shows that the Wilson lines $W_{b \rightarrow a}, W_{a \rightarrow b}, W_{d \rightarrow c}$ and $W_{e \rightarrow d} \in O(n_{\text{occ}})$ in the real, periodic basis. These Wilson lines are defined in (7.7) and (7.8).

**7.6.2 Equivalent expressions of $W[l_n(\bar{k}_z)] \in SO(n_{\text{occ}})$**

We work in a real, periodic basis where the Wilson loop $W[l_n(\bar{k}_z)] \in SO(n_{\text{occ}})$ for even $n_{\text{occ}}$, and the Wilson lines $W_{b \rightarrow a}, W_{a \rightarrow b}, W_{d \rightarrow c}$ and $W_{e \rightarrow d} \in O(n_{\text{occ}})$; cf. Sec.7.6.1. This gauge
choice is analytically convenient; note that our final result, the spectrum of the Wilson loop, is gauge-invariant. We show in this Section that all possible $W_l(\vec{k}_z)$ are classified into two groups, which are distinguished by an index $\Gamma_n(\vec{k}_z) \in \{1, -1\}$. Specifically, there exists a basis in which

$$W_l(\vec{k}_z) \sim Z^t e^{-i2\pi S/n} e^{i(1-\Gamma_n(\vec{k}_z)) M_{1,2} 2\pi/n} Z e^{i2\pi S/n}, \quad (7.20)$$

where $Z \in SO(n_{occ})$, and $\Gamma_n(\vec{k}_z) \in \{+1, -1\}$. Here, $S$ is defined

$$S = \sum_{j=1}^{n_{occ}/2} M_{2j-1,2j} \quad (7.21)$$

if the dimension of the space is $n_{occ}$, and $M_{a,b}$ are generators of rotations in the $a - b$ plane:

$$[M_{a,b}]_{ij} = -i \delta_{a,i} \delta_{b,j} + i \delta_{a,j} \delta_{b,i}, \quad (7.22)$$

for $a, b \in \{1, 2, \ldots, n_{occ}\}$. Due to the analogy with rotations in $\mathbb{R}^{n_{occ}}$, we refer to a two-dimensional subspace as a ‘plane’ in the space of occupied bands. Note that the presence of $M_{1,2}$ in (7.20) does not imply that this particular plane is special. As we will shortly clarify, by a different choice of basis (i.e., a redefinition of $Z$), one may have selected $M_{3,4}$ instead of $M_{1,2}$, or $M_{5,6}$, etc. We are interested in determining the spectrum of $W_l(\vec{k}_z)$, which is identical to the spectrum of the $SO(n_{occ})$ matrix

$$W_n(\Gamma_n) = Z^t e^{-i2\pi S/n} e^{i(1-\Gamma_n) M_{1,2} 2\pi/n} Z e^{i2\pi S/n}, \quad (7.23)$$

as follows simply from (7.20). To simplify notation, we will often suppress the dependences of various quantities on $\vec{k}_z \in \{0, \pi\}$. Before arriving at (7.20), we first derive a canonical form of the matrix representation of $C_n T$. In the basis of occupied doublet bands, the matrix is defined by

$$[V_{2\pi/n}(\vec{k})]_{ij} = \langle u_{i,-R_{2\pi/n} \vec{k}} | U_{2\pi/n} T | u_{j,\vec{k}} \rangle. \quad (7.24)$$

$R_{2\pi/n}$ implements a rotation of $2\pi/n$ in momentum space: $R_{2\pi/n}(k_x, k_y, k_z) = (k_x \cos 2\pi/n + k_y \sin 2\pi/n, k_y \cos 2\pi/n - k_x \sin 2\pi/n, k_z)$; $U_{2\pi/n}$ represents a rotation of $2\pi/n$ in the basis
of Löwdin orbitals; \( T \) is the time-reversal operator. We define \( k_i \) as \( C_n \)-invariant momenta for which \( R_{2\pi/n}(k_i) = -k_i \) up to reciprocal lattice vectors. A basis may be found where \( V_{2\pi/n}(k_i) \) has the canonical form:

\[
V_{2\pi/n}(k_i) = E(k_i) e^{i2\pi S/n} E(k_i)^t,
\]

(7.25)

where \( E(k_i) \in O(n_{occ}) \) and \( S \) is defined in (7.21). This canonical basis is both real and periodic, as defined in Sec.7.6.1. The derivation of (7.25) from (7.24) is shown in Ref. [19], for the \( C_4 + T \) insulator. We construct the canonical basis explicitly for the \( C_6 + T \) insulator.

Construction: Since the Bloch Hamiltonian is three-fold symmetric at \( k_i \), \( \{u_{n,k_i}\} \) divide into \( n_{occ}/2 \) pairs which transform in the doublet irrep of \( C_3 + T \); by assumption the singlet irreps are absent. To be explicit, let us define in each doublet subspace the basis vectors directed along \( \bar{\omega} = \frac{\pi}{n} \) and \( \bar{\omega}^* = U_{\pi/3} T |\omega\rangle \), where \( |\omega\rangle \) has \( C_3 \)-eigenvalue \( \omega = \exp[i2\pi/3] \), and \( |\omega^*\rangle \) has \( C_3 \)-eigenvalue \( \omega^* \). We form the orthogonal linear combinations: \( |1\rangle = \alpha|\omega\rangle + \beta|\omega^*\rangle \) and \( |2\rangle = -i\alpha|\omega\rangle + i\beta|\omega^*\rangle \). To satisfy (7.19), i.e., \( U_{\pi} T |1\rangle = -|1\rangle \), we set \( \alpha = -\beta^* \omega^* \). The reality condition (7.19) implies that \( [V_{\pi/3}(k_i)]_{ij} = -\langle u_{i,k_i} | U_{2\pi/3}^{-1} | u_{j,k_i} \rangle \) for \( i, j \) restricted to this doublet subspace. The projection of \( U_{2\pi/3}^{-1} \) onto this doublet subspace. The projection of \( U_{2\pi/3}^{-1} \) onto the reduced basis \( \{|1\rangle, |2\rangle\} \) is \( \exp[-i2\pi\sigma_2/3] \), where \( \sigma_2 \) is a Pauli matrix. This construction can be independently obtained within each of the \( n_{occ}/2 \) doublet subspaces. Thus we have found a canonical basis in which \( \langle u_{i,k_i} | U_{2\pi/3}^{-1} | u_{j,k_i} \rangle \) is a direct sum \( \bigoplus_{j=1}^{n_{occ}/2} \exp[-i2\pi\sigma_2/3] \), for \( n_{occ} \) occupied bands. Applying (7.21) and \( S^2 = I \), we finally derive \( V_{\pi/3}(k_i) = E(k_i) \left( -\exp[-iS2\pi/3] \right) E(k_i)^t = E(k_i) \exp[iS\pi/3] E(k_i)^t \). Now we are ready to derive (7.20); we separately tackle the \( C_6 + T \) and \( C_4 + T \) cases.

Proof of (7.20) for \( \mathcal{W}[l_0(\bar{k}_z)] \in SO(n_{occ}) \)

We recall the definitions of the \( C_3 \)-invariant momenta: \( c = (-2\pi/3, 2\pi/\sqrt{3}, k_z) \), \( d = (0, 0, k_z) \) and \( \bar{c} = (4\pi/3, 0, k_z) \), as illustrated in Fig. 7.5-(b). In the planes of constant \( \bar{k}_z \), the occupied bands \( \{u_{i,k}\} \) along the lines \( \bar{c} \searrow d \) and \( d \to c \) are related by \( C_6 T \) symmetry.
Thus from (7.8) [33],

\[ \mathcal{W}[l_0(\bar{k}_z)] = \mathcal{W}_{d\rightarrow\bar{c}} V_{\pi/3}^t \mathcal{W}_{d\rightarrow\bar{c}}^t V_{\pi/3}(c) \]  

(7.26)

and \( \mathcal{W}_{d\rightarrow\bar{c}} \in O(n_{occ}) \). Applying (7.25),

\[ \mathcal{W}[l_0(\bar{k}_z)] \sim E(c)^t \mathcal{W}_{d\rightarrow\bar{c}} E(d) e^{-iS\pi/3} E(d)^t \mathcal{W}_{d\rightarrow\bar{c}}^t E(c) e^{iS\pi/3}; \]  

(7.27)

\( \sim \) indicates an equivalence up to a unitary transformation. If \( \det[E(d)^t \mathcal{W}_{d\rightarrow\bar{c}}^t E(c)] = 1 \), we arrive at (7.20) for \( \Gamma_6 = 1 \), with the identification \( Z = E(d)^t \mathcal{W}_{d\rightarrow\bar{c}}^t E(c) \in SO(n_{occ}) \). If \( \det[E(d)^t \mathcal{W}_{d\rightarrow\bar{c}}^t E(c)] = -1 \), we employ the identity

\[ e^{-iS\pi/3} = N_2 e^{-iS\pi/3+2iM_{1,2}\pi/3} N_2^t, \]  

(7.28)

where \( N_a \) is a simple reflection with reflection axis in the direction \( a \), i.e., \( N_a \) has matrix elements

\[ [N_a]_{ij} = \delta_{ij} - 2 \delta_{a,i} \delta_{a,j}. \]  

(7.29)

(7.28) follows simply from the Clifford algebra of Pauli matrices, since \( M_{1,2} \) acts like the Pauli matrix \( \sigma_2 \) in the one-two plane, and \( N_2 \) like \( \sigma_3 \). Inserting (7.28) into (7.27) we derive (7.20) for \( \Gamma_6 = -1 \), with the identification \( Z = N_2^t E(d)^t \mathcal{W}_{d\rightarrow\bar{c}}^t E(c) \in SO(n_{occ}) \). More generally,

\[ N_a M_{b,c} = \begin{cases} M_{b,c} N_a & \text{if } a \neq b, a \neq c, \\ -M_{b,c} N_a & \text{if } a = b \text{ or } a = c. \end{cases} \]  

(7.30)

In the first case, \( M \) and \( N \) act in different subspaces; if they act in the same subspace, they anticommute. This general identity leads to

\[ e^{-iS\pi/3} = N_{2a} e^{-iS\pi/3+2iM_{2a-1,2a}\pi/3} N_{2a}^t, \]  

(7.31)

for \( a \in \{1, 2, \ldots, n_{occ}/2\} \). If we had employed this identity with \( a = 2 \), we would have derived (7.20) with \( M_{1,2} \) replaced by \( M_{3,4} \), and \( Z = N_{1}^t E(d)^t \mathcal{W}_{d\rightarrow\bar{c}}^t E(c) \). The spectrum of \( \mathcal{W} \) does not depend on this choice of plane.
Proof of (7.20) for $W[l_4(\bar{k}_z)] \in SO(n_{occ})$

We recall the definitions the $C_4$-invariant momenta: $a = (-\pi, \pi, k_z)$, $b = (0, 0, k_z)$, and $\bar{a} = (\pi, \pi, k_z)$, as illustrated in Fig. 7.5-(a). In the planes $k_z = 0$ and $\pi$, the occupied bands $\{u_{i,k}\}$ along the lines $b \nearrow \bar{a}$ and $a \searrow b$ are related by $C_4T$ symmetry. Thus from (7.7) [33],

$$W[l_4(\bar{k}_z)] = W_{b\nearrow\bar{a}} V_{\pi/2}(b)^t W_{b\nearrow\bar{a}} V_{\pi/2}(a).$$  \hspace{1cm} (7.32)

The steps leading to (7.20) are similar to those in Sec.7.6.2.

Alternative expression of $W[l_n(\bar{k}_z)] \in SO(n_{occ})$, for $n_{occ} = 4m + 2$ and integral $m$

For $n_{occ} = 4m + 2$ and integral $m$, a useful expression is:

$$W[l_n(\bar{k}_z)] \sim X^t e^{-i2\pi \Gamma_n(\bar{k}_z) S/n} X e^{i2\pi S/n} \in SO(4m + 2),$$  \hspace{1cm} (7.33)

with $X \in SO(4m + 2)$ and $\Gamma_n(\bar{k}_z) \in \{+1, -1\}$. Let us define the right-hand-side of this equation as

$$\tilde{W}_n(\Gamma_n) = X^t e^{-i2\pi \Gamma_n S/n} X e^{i2\pi S/n} \in SO(4m + 2).$$  \hspace{1cm} (7.34)

(7.33) follows directly from (7.20) if $\Gamma_n = 1$. If $\Gamma_n = -1$, we employ the identity

$$e^{-i2\pi S/n} e^{iM_{1,2}/n} = \mathcal{V} e^{i2\pi S/n} \mathcal{V}^t,$$  \hspace{1cm} (7.35)

where

$$\mathcal{V} = \mathcal{V}^t = \prod_{a=2}^{2m+1} N_{2a} \in SO(4m + 2)$$  \hspace{1cm} (7.36)

is a product of an even number of simple reflections, as defined in (7.29). (7.35) follows from applying the identity (7.30) $2m$ times, as we now show:

$$\cdots N_8 N_6 N_4 e^{i2\pi S/n} N_4^t N_6^t N_8^t \cdots$$

$$= \cdots N_8 N_6 e^{i2\pi S/n - i4\pi M_{3,4}/n} N_6^t N_8^t \cdots$$

$$= \cdots N_8 e^{i2\pi S/n - i4\pi (M_{3,4} + M_{5,6})/n} N_8^t \cdots$$  \hspace{1cm} (7.37)

Finally, we insert (7.35) into (7.20), thus obtaining (7.33) with $X = \mathcal{V}^t Z \in SO(4m + 2)$.
7.6.3 Geometric interpretation of \( W[l_n(k_z)] \in SO(n_{occ}) \)

In this Section we develop a geometric interpretation of \( W[l_n(k_z)] \in SO(n_{occ}) \) for \( n_{occ} = 2m \), and its eigenspectrum \( \{\exp(i\theta)\} \). A rotation \( R \) in \( 2m \) dimensions is described by \( m \) invariant planes, and an angle of rotation in each plane; if all \( m \) angles equal to \( \theta \), such a rotation is called equiangular. Equivalently stated, an equiangular rotation acts as \( e^{\pm i\phi_\theta} \) in each of the \( m \) invariant planes, thus there exists a basis in which \( R = e^{iJ\theta} \), where \( J = \sum_{a=1}^{n_{occ}/2} \eta_{2a-1,2a}M_{2a-1,2a} \) and \( \eta_{2a-1,2a} \in \{+1,-1\} \); \( M_{a,b} \) is the generator of rotation in the \( a-b \) plane, as defined in (7.22). From this definition, note that \( J = -J^\dagger, J = J^\dagger \) and \( J^2 = I \). We have shown that \( W[l_n(k_z)] \) is similar to (7.20), which is a product of two equiangular rotations:

\[
W_n(\Gamma_n) = R_2\left(\frac{2\pi}{n}\right) R_1\left(\frac{2\pi}{n}\right),
\]

(7.38)

where we define

\[
R_1(\phi) = e^{iS\phi}, \quad R_2(\phi) = e^{i\tilde{Y}\phi},
\]

\[
\tilde{Y} = Z^t \left[(1-\Gamma_n)M_{1,2} - S\right],
\]

(7.39)

for \( Z \in SO(n_{occ}) \). One may verify that

\[
S^2 = \tilde{Y}^2 = I, \quad S = S^\dagger, \quad \tilde{Y} = \tilde{Y}^\dagger,
\]

\[
S = -S^t \quad \text{and} \quad \tilde{Y} = -\tilde{Y}^t,
\]

(7.40)

from the definitions of \( M_{a,b} \) and \( S \) in (7.22) and (7.21). Each Berry phase is then interpreted as the net angle of rotation due to two equiangular rotations.

For any real vector \( v \), it follows from (7.40) that \( iSv \) is also real and orthogonal to \( v \). \( v \) and \( iSv \) span a plane \( \mathcal{P}_1 \) that is invariant under \( R_1 \); similarly, \( \{v, i\tilde{Y}v\} \) span a plane \( \mathcal{P}_2 \) that is invariant under \( R_2 \). It follows from (7.40) that the following norms are equal:

\[
||iSv|| = ||i\tilde{Y}v|| = ||v||.
\]

Suppose there exists a vector \( \bar{v} \) such that \( \mathcal{P}_1 \) and \( \mathcal{P}_2 \) coincide. Since both \( iS\bar{v} \) and \( i\tilde{Y}\bar{v} \) are real and have equal norms, this implies one of two cases: \( S\bar{v} = \pm \tilde{Y}\bar{v} \).
Let us define three orthogonal subspaces whose union forms the complete space.

(a) If $S\vec{v} = -\tilde{Y}\vec{v}$, $R_1$ rotates $w_+$ in a sense that is opposite to $R_2$. This is true of $w_-$ as well, hence both $w_\pm$ are invariant under $R_2R_1$, i.e., each of $w_\pm$ has eigenvalue 1. We define the invariant subspace $G_i$ as the kernel of $S + \tilde{Y}$.

(b) If $S\vec{v} = \tilde{Y}\vec{v}$, $R_1$ rotates $w_+$ in the same sense as that for $R_2$, and this is true of $w_-$ as well. Then $w_\pm$ are maximally rotated under $R_2R_1$, i.e., $w_\pm$ have eigenvalues $\exp(\pm i4\pi/n)$. We define the maximally-rotated subspace $G_m$ as the kernel of $S - \tilde{Y}$. The dimension of $G_m$ enters the weak index (7.4) as the quantity $d_n$.

(c) Since vectors in $G_m$ and $G_i$ have different eigenvalues under the same rotation, $G_m \cap G_i = 0$. $G_\perp$ is defined as the orthogonal complement to $G_i \cup G_m$. For each vector $v \in G_\perp$, the plane of rotation under $R_1$ does not coincide with the plane of rotation under $R_2$. Then $v$ is neither invariant nor maximally rotated – the net angle of rotation lies in the intermediate interval: $0 < |\vartheta| < 4\pi/n$. We had previously derived an identical bound in Sec. 7.5.1 for a product of unitary matrices, which clearly also applies for a product of equiangular rotations.

### 7.6.4 Cartan Decomposition of $SO(2m)$

Here we summarize certain ideas in the representation theory of Lie groups, which will aid in deriving the spectrum of $W[l_n(\tilde{k}_2)]$. The $SO(2m)$ group is generated by a semisimple Lie algebra $\mathcal{L}$, which can be decomposed into two subspaces: $\mathcal{L} = \mathcal{K} + \tilde{P}$. These subspaces satisfy $[\mathcal{K}, \mathcal{K}] \subseteq \mathcal{K}$, $[\mathcal{K}, \tilde{P}] \subseteq \tilde{P}$, and $[\tilde{P}, \tilde{P}] \subseteq \mathcal{K}$. Here, $[\mathcal{K}, \mathcal{K}] \subseteq \mathcal{K}$ means: if $\tilde{k}_1, \tilde{k}_2 \in \mathcal{K}$, then $[\tilde{k}_1, \tilde{k}_2] \in \mathcal{K}$. $\mathcal{K}$ is a subalgebra of $\mathcal{L}$, but $\tilde{P}$ is not. The Cartan subalgebra, as denoted by $\tilde{A}$, is defined as the maximal Abelian subalgebra that is contained in $\tilde{P}$; the dimension of $\tilde{A}$ is called the rank ($r$) of the decomposition. For an introduction to Cartan decompositions,
see Ref. [119] and references therein. Any matrix \( Z \in SO(2m) \) may be expressed as

\[
Z = e^{i\tilde{k}_1} \prod_{j=1}^{r} e^{i\Theta_j a_j} e^{i\tilde{k}_2} \in SO(2m)
\]  

(7.41)

for some real numbers \( \{\Theta_1, \Theta_2, \ldots, \Theta_r\} \). Here, \( \tilde{k}_1, \tilde{k}_2 \in K \) and \( a_j \in \tilde{A} \); \( SO(2) \) is a special case in which \( \mathcal{L} = K \). Though we are not concerned with odd spatial dimensions in this chapter, (7.41) directly generalizes the Euler parametrization of a rotation in three dimensions. Just as the Euler decomposition is very useful in representing 3D rotations, we find that the representation (7.41) reveals structure that is easily exploited, when deriving the spectrum of \( W[l_n(\bar{k}_z)] \). There are only two inequivalent types of Cartan decompositions of \( SO(2m) \), for \( m > 1 \) [120]. Their technical details are reported in the next two subsections. It is possible to skip these subsections on a first reading, and return to them when in need.

**Type-D-III Decomposition of \( SO(2m); m > 1 \)**

For a type-D-III decomposition, \( K \) is a \( U(m) \) subalgebra of \( SO(2m) \), and one choice of \( K \) is spanned by \( m^2 \) vectors:

\[
M_{2j-1,2j}, \frac{1}{2} \left( M_{2j-1,2k} + M_{2k-1,2j} \right), \quad \frac{1}{2} \left( M_{2j-1,2k-1} + M_{2j,2k} \right)
\]

(7.42)

for \( j, k \in \{1, \ldots, m\} \) and \( j \neq k \); the matrices \( M_{a,b} \) are defined in (7.22). The \( U(m) \) subalgebra contains a \( U(1) \) subalgebra which is generated by \( S \), as defined in (7.21). \( \tilde{P} \) is spanned by \( m(m-1) \) vectors:

\[
\frac{1}{2} \left( M_{2j-1,2k} - M_{2k-1,2j} \right), \quad \frac{1}{2} \left( M_{2j-1,2k-1} - M_{2j,2k} \right).
\]

(7.43)

If \( m \) is even, the rank \( r = m/2 \), and \( \tilde{A} \) is spanned by \( (M_{1+4j,4+4j} - M_{3+4j,2+4j}) \) for \( j = 0, 1, \ldots, m/2-1 \). If \( m > 1 \) and is odd, \( r = (m-1)/2 \), and \( \tilde{A} \) is spanned by \( (M_{1+4j,4+4j} - M_{3+4j,2+4j}) \) for \( j = 0, 1, \ldots, (m-1)/2 - 1 \).
Type-BD-I Decomposition of \( SO(2m); m > 1 \)

We perform a type-BD-I decomposition, where \( K \) is a \( SO(2) \times SO(2m - 2) \) subalgebra of \( SO(2m) \). One choice of \( K \) is spanned by \( M_{1,2} \) and all other \( M_{a,b} \) such that \( a, b \notin \{1, 2\} \). The subspace \( \tilde{P} \) is spanned by \( M_{1,3}, M_{1,4}, \ldots, M_{1,2m} \) and \( M_{2,3}, M_{2,4}, \ldots, M_{2,2m} \). The rank \( r = 2 \), and \( \tilde{A} \) is spanned by \( M_{1,3} \) and \( M_{2,4} \).

7.6.5 Spectrum of \( W[l_n(\bar{k}_z)] \in SO(n_{occ}) \), for specific \( \bar{k}_z \in \{0, \pi\} \)

Our aim is to prove Tab. 7.1. We know from Sec.7.6.2 that the set of all \( W[l_n(\bar{k}_z)] \in SO(n_{occ}) \) fall into two classes, which are distinguished by an index \( \Gamma_n \in \{1, -1\} \). The proof is organized into five parts: (i) In Sec.7.6.5, we solve for the spectrum of \( W[l_n(\bar{k}_z)] \in SO(2) \), i.e., with two occupied bands. (ii) In Sec.7.6.5, \( SO(4) \). (iii) In Sec.7.6.5, \( SO(4m) \) for \( m \geq 2 \) and \( \Gamma_n = 1 \). (iv) In Sec.7.6.5, \( SO(4m + 2) \) for \( m \geq 1 \). (v) Finally in Sec.7.6.5, \( SO(4m) \) for \( m \geq 2 \) and \( \Gamma_n = -1 \).

Spectrum of \( W[l_n(\bar{k}_z)] \in SO(2) \)

Applying (7.20) for two occupied bands,

\[
W[l_n(\bar{k}_z)] \sim W_n(\Gamma_n) = Z^t e^{-i\Gamma_n M_{1,2} 2\pi/n} Z e^{iM_{1,2} 2\pi/n} = e^{i(1-\Gamma_n) M_{1,2} 2\pi/n},
\]

where \( Z \in SO(2) \) and \( M_{a,b} \) is defined in (7.22). The last equality follows from the commutativity of all \( SO(2) \) matrices. If \( \Gamma_n = 1 \), the Wilson-loop spectrum is \( \{1, 1\} \); if \( \Gamma_n = -1 \), the spectrum is instead \( \{\exp(i4\pi/n), \exp(-i4\pi/n)\} \).

Spectrum of \( W[l_n(\bar{k}_z)] \in SO(4) \)

Applying (7.20) for four occupied bands,

\[
W[l_n(\bar{k}_z)] \sim W_n(\Gamma_n) = Z^t e^{-i(\Gamma_n M_{1,2} + M_{3,4}) 2\pi/n} Z e^{i(M_{1,2} + M_{3,4}) 2\pi/n},
\]

\( \text{(7.45)} \)
with $Z \in SO(4)$. The six generators of $SO(4)$ can be chosen as

\[
\begin{align*}
A_1 &= \frac{1}{2}(\tau_2 \otimes \sigma_1) \\
A_2 &= -\frac{1}{2}(\tau_2 \otimes \sigma_3) \\
A_3 &= \frac{1}{2}(\tau_0 \otimes \sigma_2) \\
B_1 &= -\frac{1}{2}(\tau_1 \otimes \sigma_2) \\
B_2 &= -\frac{1}{2}(\tau_2 \otimes \sigma_0) \\
B_3 &= \frac{1}{2}(\tau_3 \otimes \sigma_2),
\end{align*}
\]

where $\{\tau_i\}$ and $\{\sigma_i\}$ are Pauli matrices. Each of $\{A_i\}$ and $\{B_i\}$ generate an $SU(2)$ subalgebra of $SO(4)$, i.e., $[A_i, A_j] = i\epsilon_{ijk} A_k$, $[B_i, B_j] = i\epsilon_{ijk} B_k$ and $[A_i, B_j] = 0$. This is the well-known homomorphism: $SO(4) \sim SU(2) \times SU(2)$. In connection with the matrices in (7.45), we identify $M_{1,2} + M_{3,4} = 2A_3$ and $M_{1,2} - M_{3,4} = 2B_3$. Let us derive the spectrum for $\Gamma_n = \pm 1$ separately.

b.-**(i)** $\Gamma_n = 1$

A generic $SO(4)$ matrix can be written as $Z = e^{-ia \cdot A} e^{-ib \cdot B}$ for some coefficients $\{a_1, a_2, a_3, b_1, b_2, b_3\}$. Here, we treat $a = (a_1, a_2, a_3)$ as a three-vector with norm $||a|| = (a_1^2 + a_2^2 + a_3^2)^{1/2}$, and $a \cdot A = \sum_{i=1}^3 a_i A_i$. Since functions of $A$ and $B$ commute,

\[
W_n(1) = Z^t e^{-iA_3 4\pi/n} Z e^{iA_3 4\pi/n} = e^{ia \cdot A} e^{-iA_3 4\pi/n} e^{-ia \cdot A} e^{iA_3 4\pi/n} = e^{-i a' \cdot A},
\]

for some coefficients $\{a'_1, a'_2, a'_3\}$. The last equality follows from the closure property of $SU(2)$. In a basis that diagonalizes both $A_3$ and $B_3$, (7.46) is expressible as the direct product $e^{-ia' \cdot \sigma/2} \otimes I$. In this form, we identify the eigenvalues as

\[
\begin{align*}
\text{eig}[W_n(1)] &= \text{eig}[e^{-ia' \cdot \sigma/2} \otimes I] \\
&= \text{eig}\left[ \begin{pmatrix} \lambda & 0 \\ 0 & \lambda^* \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] \\
&= \{\lambda, \lambda^*, \lambda^*, \lambda^*\}.
\end{align*}
\]
Here, $\lambda$ is unimodular with phase $||a'||/2$, and we introduce eig[$\mathcal{O}$] to mean the spectrum of $\mathcal{O}$.

\[
\text{b.-(ii)} \quad \Gamma_n = -1
\]

From (7.45), we express $Z = e^{-ia^t A} e^{-ib^t B}$. Since functions of $A$ and $B$ commute,

\[
W_n(-1) = Z^t e^{iB_3 4\pi/n} Z e^{iA_3 4\pi/n}
\]

\[
= e^{ib^t B} e^{iB_3 4\pi/n} e^{-ib^t B} e^{iA_3 4\pi/n}
\]

\[
= e^{-ib^t' B} e^{iA_3 4\pi/n}, \tag{7.48}
\]

for some coefficients $\{b_1', b_2', b_3'\}$. The last equality follows from the closure property of $SU(2)$. Since $\exp(-ib^t \cdot B)$ and $\exp(i B_3 4\pi/n)$ are related by a unitary transformation, $||b'|| = 4\pi/n$. In a basis that diagonalizes both $A_3$ and $B_3$, we express (7.48) as the direct product $e^{i\sigma_3 2\pi/n} \otimes e^{-ib^t' \sigma/2}$. Then,

\[
\text{eig}[W_n(-1)] = \text{eig}[e^{i\sigma_3 2\pi/n} \otimes e^{-ib^t' \sigma/2}]
\]

\[
= \text{eig} \left[ \begin{pmatrix} e^{i2\pi/n} & 0 \\ 0 & e^{-i2\pi/n} \end{pmatrix} \otimes \begin{pmatrix} e^{i2\pi/n} & 0 \\ 0 & e^{-i2\pi/n} \end{pmatrix} \right]
\]

\[
= \{1, 1, e^{i4\pi/n}, e^{-i4\pi/n}\}. \tag{7.49}
\]

**Spectrum of $W[l_n(\bar{k}_z)] \in SO(4m); \ m \geq 2; \ \Gamma_n = 1$**

We employ the form of $W[l_n(\bar{k}_z)] \in SO(4m)$ in (7.20), for $\Gamma_n = 1$. Following Sec.7.6.4, we perform a type-D-III Cartan decomposition of the matrix $Z$ in (7.20), i.e., we express $Z$ in the form (7.41) for some coefficients $\{\Theta_1, \Theta_2, \ldots, \Theta_r\}$; the rank of the decomposition $r = m$; $\{\tilde{k}_1, \tilde{k}_2\}$ belong to a $U(2m)$ subalgebra ($\mathcal{K}$) of $SO(4m)$. The Cartan subalgebra is spanned by

\[
a_j = \frac{1}{2} \left( M_{4j-3,4j} - M_{4j-1,4j-2} \right) \tag{7.50}
\]
for \( j \in \{1, 2, \ldots, m\} \). As defined in (7.21), the matrix \( S \) of (7.20) generates a \( U(1) \) subalgebra in \( K \), i.e., it commutes with all elements in the \( U(2m) \) subgroup generated by \( K \). Hence, (7.20) simplifies to

\[
\mathcal{W}_n(1) \sim \prod_{j=1}^{m} e^{-i\Theta_j a_j} e^{-2\pi S/n} \prod_{u=1}^{m} e^{i\Theta_u a_u} e^{2\pi S/n} \tag{7.51}
\]

in some basis. Now insert the identity:

\[
e^{2\pi S/n} = \prod_{j=1}^{m} e^{i(M_{4j-3,4j-2} + M_{4j-1,4j}) 2\pi/n}, \tag{7.52}
\]

which follows simply from (7.21). Let us denote the basis vectors by \( \{v_i | i \in \{1, 2, \ldots, 4m\}\} \). We define \( \mathcal{N}(j) \) as the 4D subspace spanned by \( v_{4j-3}, v_{4j-2}, v_{4j-1} \) and \( v_{4j} \). Since \( a_j \) and \( M_{4j-3,4j-2} + M_{4j-1,4j} \) act only in \( \mathcal{N}(j) \), we may arrange (7.51) as

\[
\mathcal{W}_n(1) \sim \prod_{j=1}^{m} \left( e^{-i\Theta_j a_j} e^{-i(M_{4j-3,4j-2} + M_{4j-1,4j}) 2\pi/n} \times e^{i\Theta_j a_j} e^{i(M_{4j-3,4j-2} + M_{4j-1,4j}) 2\pi/n} \right) = \bigoplus_{j=1}^{m} Q^{(j)}. \tag{7.53}
\]

Equivalently, \( \mathcal{W}_n(1) \) diagonalizes into \( m \) blocks – each block \( Q^{(j)} \in SO(4) \) acts in the subspace of \( \mathcal{N}(j) \). We proceed to determine the eigenvalues within each block \( Q^{(j)} \). First, we show that \( a_j \) and \( M_{4j-3,4j-2} + M_{4j-1,4j} \) generate an \( SU(2) \) subalgebra in \( \mathcal{N}(j) \). The six generators of \( SO(4) \) in each block may be chosen as

\[
\begin{align*}
A_1^{(j)} &= a_j = \frac{1}{2} \left( M_{4j-3,4j} - M_{4j-1,4j-2} \right) \\
A_2^{(j)} &= \frac{1}{2} \left( M_{4j-2,4j} - M_{4j-3,4j-1} \right) \\
A_3^{(j)} &= \frac{1}{2} \left( M_{4j-3,4j-2} + M_{4j-1,4j} \right) \\
B_1^{(j)} &= -\frac{1}{2} \left( M_{4j-3,4j} + M_{4j-1,4j-2} \right) \\
B_2^{(j)} &= -\frac{1}{2} \left( M_{4j-2,4j} + M_{4j-3,4j-1} \right) \\
B_3^{(j)} &= \frac{1}{2} \left( M_{4j-3,4j-2} - M_{4j-1,4j} \right). \tag{7.54}
\end{align*}
\]

Each of \( \{A_i^{(j)}\} \) and \( \{B_i^{(j)}\} \) generate an \( SU(2) \) subalgebra of \( SO(4) \), i.e., they satisfy
\[
[A_i^{(j)}, A_m^{(j)}] = i \epsilon_{lmn} A_n^{(j)},
\]
\[
[B_i^{(j)}, B_m^{(j)}] = i \epsilon_{lmn} B_n^{(j)},
\]
and
\[
[A_i^{(j)}, B_m^{(j)}] = 0.
\]
Thus, we identify \( Q^{(j)} \) as an element in the \( SU(2) \) subgroup generated by \( \{A_i^{(j)}\} \). The spectrum in each of \( Q^{(j)} \) has been solved in Sec.7.6.5 – the full spectrum comprises \( m \) sets of complex-conjugate quartets:
\[
\text{eig}[W_n(1)] = \{ \lambda_1, \lambda_1^*, \lambda_1^*, \ldots, \lambda_m, \lambda_m^*, \lambda_m^*, \lambda_m^* \}.
\]

**Spectrum of** \( W[l_n(k_z)] \in SO(4m+2) \), **for** \( m \geq 1 \)

We employ the form of \( W[l_n(k_z)] \in SO(4m+2) \) in (7.33). Following Sec.7.6.4, we perform a type-D-III Cartan decomposition of the matrix \( X \) in (7.33), i.e., we express \( X \) in the form (7.41) for some \( \{\Theta_1, \Theta_2, \ldots, \Theta_r\} \); the rank of the decomposition \( r = m \); \( \{\bar{k}_1, \bar{k}_2\} \) belong to a \( U(2m+1) \) subalgebra (\( \mathcal{K} \)) of \( SO(4m+2) \). The Cartan subalgebra is spanned by (7.50).

As defined in (7.21), the matrix \( S \) in (7.33) commutes with all elements generated by \( \mathcal{K} \), hence (7.33) simplifies to
\[
\tilde{W}_n(\Gamma_n) \sim \prod_{l=1}^{m} e^{-i\Theta_la_l} e^{-i2\pi \Gamma_n S/n} \prod_{l=1}^{m} e^{i\Theta_la_l} e^{i2\pi S/n}.
\]

Let us denote the basis vectors by \( \{v_i | i \in \{1, 2, \ldots, 4m+2\} \} \), and the plane spanned by \( v_i \) and \( v_j \) as \( \mathcal{P}_{ij} \). We consider the cases \( \Gamma_n = \pm 1 \) separately.

\[
d.-(i) \quad \Gamma_n = 1
\]

In the basis of (7.56), any vector \( \bar{v} \in \mathcal{P}_{4m+1,4m+2} \) is invariant under \( \tilde{W}_n(1) \). Thus there are at least two unit eigenvalues in the spectrum of \( \tilde{W}_n(1) \).

**Proof**: As defined in (7.50), \( a_j \) generates rotations in the planes \( \mathcal{P}_{4j-3,4j} \) and \( \mathcal{P}_{4j-1,4j-2} \), thus any vector in \( \mathcal{P}_{4m+1,4m+2} \) is invariant under the rotation \( \prod_{j=1}^{m} \exp(i\Theta_ja_j) \). Moreover, any rotation of \( \bar{v} \) that is induced by \( \exp(iS2\pi/n) \) is subsequently negated by \( \exp(-iS2\pi/n) \).
Within the orthogonal complement of \( P_{4m+1,4m+2} \), each \( a_j \) acts in \( \mathcal{N}^{(j)} \), defined as the 4D subspace spanned by \( v_{4j-3}, v_{4j-2}, v_{4j-1} \) and \( v_{4j} \). Therefore, \( \tilde{W}_n(1) \) diagonalizes into (i) two one-by-one blocks with unit element, in the plane \( P_{4m+1,4m+2} \), and (ii) \( m \) four-by-four blocks, each labelled by \( Q^{(j)} \in SO(4) \): 
\[
\tilde{W}_n(1) = I_{2 \times 2} \oplus \bigoplus_{j=1}^{m} Q^{(j)}.
\]
The spectrum in each of \( Q^{(j)} \) has been solved in Sec.7.6.5 – the full spectrum is
\[
\text{eig}[\tilde{W}_n(1)] = \{ 1, 1, \lambda_1, \lambda_1^*, \lambda_1^*, \ldots, \lambda_m, \lambda_m, \lambda_m^*, \lambda_m^* \}. \tag{7.57}
\]

\( d.-(ii) \quad \Gamma_n = -1 \)

A vector \( \vec{v} \in P_{4m+1,4m+2} \) is (i) invariant under \( \prod_{j=1}^{m} \exp(i \Theta_j a_j) \), but (ii) is rotated by \( 4\pi/n \) due to a double application of \( \exp(i 2\pi S/n) \). The remainder of the proof is similar to the case of \( \Gamma_n = +1 \). We conclude that the full spectrum is
\[
\text{eig}[\tilde{W}_n(-1)] = \{ e^{i 4\pi/n}, e^{-i 4\pi/n}, \lambda_1, \lambda_1^*, \lambda_1^*, \lambda_1^*, \ldots, \lambda_m, \lambda_m^*, \lambda_m^* \}. \tag{7.58}
\]

**Spectrum of** \( W[l_n(\vec{k}_z)] \in SO(4m) \), **for** \( m \geq 2 \) **and** \( \Gamma_n = -1 \)

We employ the form of \( W[l_n(\vec{k}_z)] \in SO(4m) \) in (7.20), for \( \Gamma_n = -1 \), i.e., a basis is found where \( W[l_n(\vec{k}_z)] \sim W_n(-1) \). Some useful notations are defined in Sec.7.6.3: \( R_1(\phi) = \exp(iS\phi) \) and \( R_2(\phi) = \exp(i\tilde{Y} \phi) \); \( Y = 2M_{1,2} - S \) and \( \tilde{Y} = Z^t Y Z \) for \( Z \in SO(4m) \). \( M_{ab} \) and \( S \) are defined in (7.22) and (7.21). We first solve for the spectrum of \( W_4(-1) \in SO(4m) \).

\( e.-(i) \quad \text{Spectrum of} \ W_4(-1) \in SO(4m), \text{for} \ m \geq 2 \)

For the \( C_4 + T \) insulator, \( W_4(-1) = R_2(\frac{\pi}{2}) R_1(\frac{\pi}{2}) = i \tilde{Y} i S \). We first derive two general properties of its spectrum:
(i) Since $\mathcal{W}_4(-1)$ is a proper rotation in even dimensions, its spectrum comprises of complex-conjugate pairs.

(ii) Moreover, there exists an antiunitary operator $\mathcal{O} = i S \hat{K}$, where $\hat{K}$ implements complex-conjugation, such that

$$
\mathcal{O} \mathcal{W}_4(-1) \mathcal{O}^{-1} = i S i \hat{Y} = \mathcal{W}_4(-1)^t = \mathcal{W}_4(-1)^{-1}.
$$

(7.59)

Here, we applied that $S$ and $\hat{Y}$ are each imaginary and skew-symmetric; cf. (7.40). Since $\mathcal{O}^2 = -I$, (7.59) implies that each eigenvalue of $\mathcal{W}_4(-1)$ is doubly-degenerate [33].

Following Sec.7.6.4, we perform a type-BD-I Cartan decomposition of $Z$ in $\hat{Y} = Z^t Y Z$, i.e., we express $Z$ in the form (7.41) for some $\{\Theta_1, \Theta_2\}$; the rank of the decomposition $r = 2$; $\{\tilde{k}_1, \tilde{k}_2\}$ belong to a $SO(2) \times SO(4m - 2)$ subalgebra ($\mathcal{K}$) of $SO(4m)$. The Cartan subalgebra is spanned by the generators $a_1 = M_{1,3}$ and $a_2 = M_{2,4}$, where $[a_1, a_2] = 0$. Our strategy is to derive the spectrum for the special values $\Theta_1 = \Theta_2 = 0$, and then prove that the spectrum for arbitrary $(\Theta_1, \Theta_2)$ has essentially the same structure. If $\Theta_1 = \Theta_2 = 0$,

$$
\mathcal{W}_4(-1) = e^{-i\tilde{k}_3} i Y e^{i\tilde{k}_3} i S
$$

(7.60)

where $\exp(i\tilde{k}_3) = \exp(i\tilde{k}_1) \exp(i\tilde{k}_2)$ for some $\tilde{k}_3 \in \mathcal{K}$, due to the closure property of the subgroup generated by $\mathcal{K}$. Let us define $\mathcal{P}_{12}$ as the plane spanned by basis vector $v_1$ and $v_2$. Since none of $\mathcal{K}$, $Y$ and $S$ couple $\mathcal{P}_{12}$ to its orthogonal complement, $\mathcal{W}_4(-1)$ diagonalizes into two blocks, with dimensions 2 and $(4m - 2)$. The two-dimensional block has the form (7.44) for $n = 4$ and $\Gamma_4 = -1$, so we may apply the results derived in Sec.7.6.5 – the spectrum in this block is $\{-1, -1\}$. The $(4m - 2)$-dimensional block has the form (7.33) for $n = 4$ and $\Gamma_4 = +1$; take care that the integer $m$ in this Section differs from that of (7.33) by unity. We then apply the results derived in Sec.7.6.5 for $\Gamma_4 = +1$ – the spectrum in this block is $\{1, 1, \lambda_1, \lambda_1^*, \lambda_1^*, \ldots, \lambda_{m-1}, \lambda_{m-1}, \lambda_{m-1}^*, \lambda_{m-1}^*\}$. The full spectrum for $\Theta_1 = \Theta_2 = 0$ is
thus
\[
\text{eig}[W_4(-1)] = \{ -1, -1, 1, 1, \lambda_1, \lambda_1^*, \ldots, \\
\lambda_{m-1}, \lambda_{m-1}^*, \lambda_{m-1}^* \}.
\] (7.61)

Since $Z$ is analytic in both $\Theta_1$ and $\Theta_2$, so is the operator $W_4(-1)$. This implies that the eigenvalues of $W_4(-1)$ are continuous functions of $\Theta_1$ and $\Theta_2$ [121,122]. Thus we consider interpolating between $(\Theta_1, \Theta_2) = (0,0)$ to any values which can be nonzero. We note that the properties (i) and (ii) of the above discussion were derived for the most general form of the matrix $Z$, i.e., they are applicable for any value of $\Theta_1$ and $\Theta_2$. Together, (i) and (ii) imply that any eigenvalue that is not $\pm 1$ must belong to a complex-conjugate quartet: $\{\lambda, \lambda, \lambda^*, \lambda^*\}$ – this is true throughout the interpolation. We have derived that the spectrum at $\Theta_1 = \Theta_2 = 0$ comprises two eigenvalues at $+1$ and the two eigenvalues at $-1$; in the interpolation, these four eigenvalues cannot combine to form a complex-conjugate quartet in any continuous fashion, hence they are invariants of the interpolation. Thus we have shown that spectrum of $W_4(-1)$ for any finite $(\Theta_1, \Theta_2)$ has the same form as that in (7.61). In particular, we have shown that there are at least 2 eigenvalues of $+1$; it is possible that one or more of the complex-conjugate quartets lie at $+1$ as well, hence the total number is more generally $2 + 4t$, for $t$ a non-negative integer less than $m$. Similarly, the number of $-1$ eigenvalues might be $2 + 4u$, for $u$ a non-negative integer less than $m$; $u + t < m$. We proceed to evaluate the spectrum of $W_6(-1) \in SO(4m)$ for the $C_6 + T$ insulator.

e.-(ii) Spectrum of $W_6(-1) \in SO(4m)$, for $m \geq 2$

**Lemma 1**: the spectrum of $W_6(-1)$ consists of: (i) $2 + 4u$ number of $+1$ eigenvalues, and (ii) $1 + 2t$ pairs of $\exp(\pm 2\pi/3)$, for some non-negative integers $u$ and $t$ that satisfy $u + t < m$.

**Proof**: Though we are interested in the spectrum of $W_6(-1) = R_2(\pi/3) R_1(\pi/3)$, let us first consider the more general problem of
\[
W(\phi) = R_2(\phi) R_1(\phi); \quad 2|\phi| \leq \pi.
\] (7.62)
As introduced in Sec. 7.6.3, \( \mathbb{R}^{4m} \) may be divided into three orthogonal subspaces:

\[
G_i = \ker [ S + \tilde{Y} ], \quad G_m = \ker [ S - \tilde{Y} ], \\
\text{and} \quad G^\perp = \mathbb{R}^{4m} \setminus (G_i \cup G_m). \tag{7.63}
\]

Here, \( \ker [O] \) means the kernel of the operator \( O \). An eigenvector of \( W(\phi) \) in the invariant subspace \( G_i \) has unit eigenvalue; in the maximally-rotated subspace \( G_m \), the eigenvalues appear in pairs of \( \exp(\pm i 2\phi) \). The decomposition (7.63) is manifestly independent of \( \phi \).

This suggests the following strategy: evaluate \( G_i \) and \( G_m \) for \( W(\phi) \) with \( \phi \neq \pi/3 \); these subspaces must be identical for the matrix \( W(\pi/3) = W_6(-1) \). Conveniently, we apply the result (7.61), for \( W_4(-1) = W_6(\pi/2) \). In the case of \( \phi = \pi/2 \), we have derived that there are \( 2 + 4t \) \((2 + 4u)\) number of \(+1\) \((-1)\) eigenvalues, for some non-negative integers \( \{u, t\} \) which satisfy \( u + t < m \). It follows that the dimension of \( G_i \), denoted by \( \dim[G_i] \), equals \( 2 + 4t \), and \( \dim[G_m] = 2 + 4u \). This proves Lemma 1.

We proceed to evaluate the spectrum of \( W_6(-1) \) in the subspace \( G^\perp \), in the case that \( \dim[G^\perp] = 4(m - 1 - t - u) \) is nonzero. **Lemma 2**: the spectrum comprises \( \dim[G^\perp]/4 \) sets of complex-conjugate quartets: \( \{\lambda_i, \lambda_i^*, \lambda_i^*, \lambda_i^*\} \).

**Proof**: Let us show that \( G = G_m \cup G_i \) is spanned by the simultaneous eigenvectors of \( \tilde{Y} \) and \( S \). For any \( v \in G_m \), the orthogonal linear combinations \( w_\pm = v \pm Sv \in G_m \) satisfy \( Sw_\pm = \tilde{Y} w_\pm = \pm w_\pm \). Similarly, for any \( y \in G_i \), the orthogonal linear combinations \( z_\pm = y \pm Sy \in G_i \) satisfy \( Sz_\pm = -\tilde{Y} z_\pm = \pm z_\pm \). Denoting the projection to a subspace \( \mathcal{C} \) by \( P(\mathcal{C}) \), it follows that

\[
[P(\mathcal{G}), S] = [P(\mathcal{G}), \tilde{Y}] = 0 \\
\Rightarrow P(\mathcal{G}) R_2(\frac{\pi}{3}) P(\mathcal{G}^\perp) = P(\mathcal{G}) R_1(\frac{\pi}{3}) P(\mathcal{G}^\perp) = 0 \\
\Rightarrow P(\mathcal{G}^\perp) W_6(-1) P(\mathcal{G}^\perp) = \left( P(\mathcal{G}^\perp) R_2(\frac{\pi}{3}) P(\mathcal{G}^\perp) \right) \times \left( P(\mathcal{G}^\perp) R_1(\frac{\pi}{3}) P(\mathcal{G}^\perp) \right) \tag{7.64}
\]
Alternatively stated, $G^\perp$ is closed under the operations $R_2$ and $R_1$. This implies that $P(G^\perp) R_1(\pi/3) P(G^\perp)$ remains an equiangular rotation in spite of the projection, i.e., there exists a reduced basis where this operator is represented by $\exp(iJ\pi/3) \in SO(\dim[G^\perp])$, for a generator that satisfies $J = J^\dagger$, $J^2 = I$ and $J = -J^t$. Similarly, $P(G^\perp) R_2(\pi/3) P(G^\perp)$ is also an equiangular rotation in this reduced basis. A product of two equiangular rotations has the form (7.20) in a suitably chosen basis for $G^\perp$:

$$P(G^\perp) W_6(-1) P(G^\perp) \sim B^t e^{-iS_{\perp} \pi/3} e^{i(1-\gamma)} M_{2,\perp}^{\perp} \pi/3 B e^{iS_{\perp} \pi/3},$$

(7.65)

where $B \in SO(\dim[G^\perp])$. $S_{\perp}$ and $M_{a,b}^{\perp}$ are to be distinguished from $S$ and $M_{a,b}$, which appear in the earlier discussion. Though they share similar definitions in (7.21) and (7.22), they are defined on different bases: $S_{\perp}$ and $M_{a,b}^{\perp}$ are linear operators in $G^\perp$, while $S$ and $M_{a,b}$ are linear operators in $G \cup G^\perp$. The form (7.20) is general and does not specify whether $\gamma = +1$ or $-1$. Now we prove that our case (7.65) corresponds to $\gamma = +1$. Suppose $\gamma = -1$, then we may apply Lemma 1 in the reduced subspace $G^\perp$. We conclude that $P(G^\perp) W_6(-1) P(G^\perp)$ has at least the eigenvalues $\{1, 1, e^{i2\pi/3}, e^{-i2\pi/3}\}$. We have shown in Sec.7.6.3 that the eigenvalues $\{\exp(i\vartheta)\}$ of $G^\perp$ satisfy $0 < |\vartheta| < 2\pi/3$, if $\vartheta$ is defined on the branch $-\pi < \vartheta \leq \pi$. Thus we arrive at a contradiction. What remains is $\gamma = +1$. We have solved the eigenspectrum for such a case in Sec.7.6.5: we obtain $\dim[G^\perp]/4$ sets of complex-conjugate quartets: $\{\lambda_i, \lambda_i^*, \lambda_1^*, \lambda_1\}$, as desired.

Combining Lemmas 1 and 2, the full spectrum is

$$\text{eig}[ W_6(-1) ] = \{ e^{i2\pi/3}, e^{-i2\pi/3}, 1, 1, \lambda_1, \lambda_1^*, \lambda_1^*, \ldots, \lambda_{m-1}, \lambda_{m-1}, \lambda_{m-1}^*, \lambda_{m-1}^* \}.$$  

(7.66)

This completes the proof of Tab. 7.1.
7.7 Alternative expression of the Wilson-loop index $\Gamma_n(\bar{k}_z)$

The weak index was first formulated in Ref. [19] as an invariant involving the Pfaffian of a matrix. In this Section we show that the Pfaffian formulation is equivalent to the Wilson-loop index $\Gamma_4$ for the $C_4 + T$ insulator. $\Gamma_6$ is also equivalent to a Pfaffian invariant, though the proposed formula in Ref. [19] requires a clarification.

7.7.1 The $C_6 + T$ insulator

Let $V_{\pi/3}(k)$ be the matrix representation of $C_6 T$ in the basis of occupied doublet bands, as defined in (7.24). Let $k_s$ denote momenta which are invariant under $C_6 T$, i.e., $-R_{2\pi/3}k_s = k_s$ up to a reciprocal lattice vector. These include the momenta $\Gamma, K, A$, and $H$ of Fig. 3.6(b). It should be noted that $V_{\pi/3}(k_s)$ is not skew-symmetric, thus the proposed formula (Eq. (6) in Ref. [19]) for the $C_4 + T$ case cannot immediately be generalized to $C_6 + T$. Instead, we define $V_{\pi/3}^a(k_s) = (V_{\pi/3}(k_s) - V_{\pi/3}(k_s)')/2$ as the skew-symmetric part of $V_{\pi/3}$.

The Wilson-loop index in the $k_z = 0$ plane is alternatively expressed as

$$\Gamma_6(0) = e^{\int K} \text{Tr}[A(k)] - \text{d}k \frac{\text{Pf}[V_{\pi/3}^a(\Gamma)]}{\text{Pf}[V_{\pi/3}^a(K)]},$$

(7.67)

where Pf denotes the Pfaffian,

$$\text{Tr}[A(k)] = \sum_{i=1}^{n_{\text{occ}}} \langle u_{i,k} | \nabla_k | u_{i,k} \rangle$$

(7.68)

is the Abelian Berry connection, and the integral follows an arbitrary path that connects $K$ to $\Gamma$. Under gauge transformations: $|u_{i,k}\rangle \to \sum_j |u_{j,k}\rangle U(k)_{ji}$ for $U(k) \in U(n_{\text{occ}})$, $V^a \to U(k_s)^\dagger V^a U(k_s)^*$ which is manifestly skew-symmetric. Alternatively stated, the symmetric and anti-symmetric components of $V_{\pi/3}(k_s)$ do not mix under gauge transformations. It follows that the entire expression on the right-hand-side (RHS) of (7.67) is gauge-invariant [19].

Proof of (7.67): Let us pick the shortest path that connects $K$ to $\Gamma$, in the positive quadrant
of the \( k_z = 0 \) plane. Then we relate

\[
e^{\int_{\Gamma}^{\Lambda} \text{Tr}[A(k)] \, dk} = \det[\mathcal{W}_{d\rightarrow \bar{c}}], \tag{7.69}
\]

where \( \mathcal{W}_{d\rightarrow \bar{c}} \) is a Wilson line defined in Sec. 7.4. In the real, periodic basis of (7.6.1), \( \mathcal{W}_{d\rightarrow \bar{c}} \in O(n_{occ}) \) and the matrix \( V_{\pi/3} \) is chosen to have the canonical form (7.25), thus

\[
V_{\pi/3}^a(k_s) = \sin (\pi/3) E(k_s) i S E(k_s)^t, \tag{7.70}
\]

where \( E(k_s) \in O(n_{occ}) \) and \( S \) is defined in (7.21). Exploiting the identity \( \text{Pf}[E(k_s) i S E(k_s)^t] = \det[E(k_s)] \), we derive

\[
e^{\int_{\Gamma}^{\Lambda} \text{Tr}[A(k)] \, dk} \frac{\text{Pf}[V_{\pi/3}^a(\Gamma)]}{\text{Pf}[V_{\pi/3}^a(K)]} = \det[E(d) \mathcal{W}_{d\rightarrow \bar{c}} E(c)^t] \in \{1, -1\}. \tag{7.71}
\]

In Sec. 7.6.2, we identify \( \Gamma_6(0) = \det[E(d) \mathcal{W}_{d\rightarrow \bar{c}} E(c)^t] \).

### 7.7.2 The \( C_4 + T \) insulator

Let \( V_{\pi/2}(k) \) be the matrix representation of \( C_4 T \) in the basis of occupied doublet bands, as defined in (7.24). Let \( k_s \) denote momenta which are invariant under \( C_4 T \), i.e., \(-R_{\pi/2}k_s = k_s\) up to a reciprocal lattice vector; these include the momenta \( \Gamma, M, Z, \) and \( A \) of Fig. 3.6(a). It should be noted that \( V_{\pi/2}(k_s) \) is skew-symmetric [19]. The Wilson-loop index in the \( k_z = 0 \) plane is alternatively expressed as

\[
\Gamma_4(0) = e^{\int_{M}^{\Gamma} \text{Tr}[A(k)] \, dk} \frac{\text{Pf}[V_{\pi/2}(\Gamma)]}{\text{Pf}[V_{\pi/2}(M)]}, \tag{7.72}
\]

where the integral follows an arbitrary path that connects \( M \) to \( \Gamma \). The RHS of (7.72) is gauge-invariant [19].

**Proof of (7.72):** The steps are closely analogous to the \( C_6 + T \) case. Let us pick the shortest path that connects \( M \) to \( \Gamma \), in the positive quadrant of the \( k_z = 0 \) plane. Then we relate

\[
e^{\int_{M}^{\Gamma} \text{Tr}[A(k)] \, dk} = \det[\mathcal{W}_{b\rightarrow a}], \tag{7.73}
\]
where $W_{b,\gamma}$ is a Wilson line defined in Sec. 7.4. A basis is found where $V_{\pi/2}$ has the canonical form (7.25), or equivalently,

$$V_{\pi/2}(k_s) = E(k_s) i S E(k_s)^t; \quad E(k_s) \in O(n_{occ}).$$

(7.74)

It follows that

$$e^{\int_M^\Gamma Tr[A(k)]} dk \frac{\text{Pf}[V_{\pi/2}(\Gamma)]}{\text{Pf}[V_{\pi/2}(M)]} = \det[E(b) W_{b,\gamma} E(a)^t] \in \{1, -1\}. (7.75)$$

In Sec. 7.6.2, we identify

$$\Gamma_4(0) = \det[E(b) W_{b,\gamma} E(a)^t]. (7.76)$$

7.8 Choice of spatial origin for the bent Wilson loop

As shown in Sec. 2.4, translating the spatial origin multiplies each Berry-Zak phase by a global $U(1)$ phase. Consider then the implications of this $U(1)$ variance on the bent Wilson loop $\hat{W}[l_4(\bar{k}_z)]$, for $\bar{k}_z \in \{0, \pi\}$ and the loop $l_4(\bar{k}_z)$ defined in Sec. 7.2. For example, $l_4(0)$ is the loop connecting $M - \Gamma - M$ in the $k_z = 0$ plane, as depicted in red in Fig. 7.1(a); to be explicit, we may choose coordinates such that the loop starts at $k(0) = M$ and ends at $k^{(o)} + G = M + 2\pi\hat{x}/a$, with $a$ a lattice constant in the tetragonal lattice. As an example, we consider a tetragonal lattice composed of two interpenetrating sublattices, which are correspondingly colored red and blue in Fig. 7.2(a). We label our orbital basis by $\alpha = 1$ (resp. 2) for $p_x + ip_y$ (resp. $p_x - ip_y$) orbitals on the blue sublattice, and $\alpha = 3$ (resp. 4) for $p_x - ip_y$ (resp. $p_x + ip_y$) orbitals on the red sublattice. Suppose the spatial origin lies on an atomic site in the blue sublattice, e.g., the corner of the cube in Fig. 7.2(a). With this choice of origin, the spatial embeddings are $r_1 = r_2 = 0$, and $r_3 = r_4 = \Delta \hat{z}$ corresponds to the vertical offset between the two sublattices – clearly, with $G = 2\pi\hat{x}/a$, the phase factor $e^{iG \cdot r_\alpha}$ is trivially unity for all $\alpha$. In Sec. 7.2, we defined the trivial (resp. weak) phase by their Berry-Zak spectrum: $\mathcal{W}[l_4(0)] = \mathcal{W}[l_4(\pi)] = +I$ (resp. $-I$). We point out that this definition is only meaningful if we specify the spatial origin, which in this case lies on an atomic
site. There exists a second choice of origin that manifests the four-fold rotational symmetry, e.g., the cross in Fig. 7.2(a) and (b). With this second choice, \( r_1 = r_2 = a(\hat{x} + \hat{y})/2 \) (illustrated by the green arrow in Fig. 7.2(b)), and \( r_3 = r_4 = a(\hat{x} + \hat{y})/2 + \Delta \hat{z} \). Now the phase factor \( e^{i G \cdot r_\alpha} = -1 \) for all \( \alpha \), and the same trivial (resp. weak) phase is characterized by \( \mathcal{W}[l_4(0)] = \mathcal{W}[l_4(\pi)] = -I \) (resp. +I).

Independent of the choice of origin, we note that: (i) the strong phase is always uniquely characterized by spectral flow, and (ii) the trivial and weak phases always differ in their Berry phases, when the comparison is made with the same choice of origin; this difference is measurable in principle, e.g., by generalizing the cold-atom experiment performed in Ref. [82]. It is also possible to formulate the weak indices such that they are invariant under translations of the origin, as we now elaborate. A simple resolution is consider the modified Wilson loop \( e^{-i G \cdot r_1 \hat{W}[l_4(\vec{k}_z)]} \). This modified operator coincides with \( \hat{W}[l_4(\vec{k}_z)] \) if the spatial origin lies on the atomic site; by construction, the eigenspectrum of \( e^{-i G \cdot r_1 \hat{W}[l_4(\vec{k}_z)]} \) does not change if we displace the origin. Then we define \( d_4(\vec{k}_z) \) as the number of \(-1\) eigenvalues of this modified Wilson loop, and similarly define the weak index through (7.4).

### 7.9 Conclusion

The geometric theory of polarization has wide applications in topological band theory. [33, 71, 78] This Chapter points out that some Berry-Zak phases have no interpretation in terms of polarization, but they are nevertheless interesting characterizations of band insulators. We have shown that bent Wilson loops distinguish a class of time-reversal-invariant topological phases with the \( C_n \) point-group symmetry; some of these phases do not have robust surface modes, but are experimentally distinguishable by their Berry-Zak phases.
Part IV

Summary and Outlook

A final remark regards a general methodology to topologically classify band insulators. In many cases, one may infer the classification purely from the representation theory [36,62,72] of surface wavefunctions. We have identified a criterion on the surface-symmetry representations that applies to all known symmetry-protected surface topologies, and presumably to some unknown ones as well. By ‘symmetry-protected’, we refer to nonchiral surface states that have vanishing Chern [2] (or mirror Chern [34]) numbers. Our criterion introduces the notion of connectivity within a submanifold (\(M\)) of the surface Brillouin zone, and relates to the theory of elementary band representations [20, 21] – we say there is a \(D\)-fold connectivity within \(M\) if bands here divide into sets of \(D\), such that within each set there are enough contact points in \(M\) to continuously travel through all \(D\) branches. If \(M\) is a single wavevector \((k_\parallel)\), \(D\) coincides with the dimension of the irreducible representation at \(k_\parallel\); \(D\) generalizes this notion of symmetry-enforced degeneracy where \(M\) is larger than a wavevector (e.g., a glide line). We are ready to state our criterion: (a) there exist two separated submanifolds \(M_1\) and \(M_2\), with corresponding \(D_1=\ldots=D_2=fd\) (\(f\geq2\) and \(d\geq1\) are integers), and (b) a third submanifold \(M_3\) that connects \(M_1\) and \(M_2\), with corresponding \(D_3=d\). Almost all symmetry-protected surface topologies [3,19,36,62,72] are characterized by \(D_1=\ldots=D_2=2D_3=2\), with \(M_1\) and \(M_2\) two high-symmetry wavevectors that are connected by a curve \(M_3\). A case in point would be symmorphic \(C_{nv}\) groups, whose topology we
studied in Chap. 3. We also investigated a non-symmorphic surface symmetry \((Pma2)\) in Chap. 4; this group is characterized by two glide lines \((M_1=\bar{\Gamma}\bar{Z}, M_2=\bar{X}\bar{U})\) with hourglass bandstructures \((D_1=D_2=4)\), and a normal mirror line \((M_3=\bar{Z}\bar{U})\) with doubly-degenerate bands \((D_3=2)\). Previous studies of magnetic systems \([65,66]\) have established a \(Z_2\) topology with \(D_1=D_2=2D_3=2\), where \(M_1\) and \(M_2\) are also parallel glide lines.

This surface-centric approach is technically simple, and has proven to be predictive of the topological classification. However, we also found it to be over-predictive, in the sense of anticipating some topologies that are inconsistent with the full set of bulk symmetries. In the \(C_{nv}\) case, a reflection \((M_z)\) axis that is parallel to the principal rotation axis would disable the half-mirror topology; for \(Pma2\), the out-of-surface translational symmetry \((t_\perp)\) was found in Chap. 5 to disable a glide-spin-Hall topology. Both \(M_z\) and \(t_\perp\) are bulk symmetries that are spoilt by the surface, but they are encoded in the Wilson loop – a representation theory for Wilson loops is thus more fundamental in band topology. Indeed, the elementary-band criterion described in the previous paragraph may also be applied to the Wilson ‘bands’, which disperse as a function of a surface wavevector – such a Wilson-centric approach is sure-fire in finding nontrivial topologies, as we illustrated in Chap. 5. To determine the possible Wilson ‘bandstructures’, one has to determine how symmetries are represented in the Wilson loop; one lesson learned in Chap. 5 is that this representation is sometimes projective. A projective representation here corresponds to an un-split extension of the crystal group by Wilson loops (or quasimomentum translations). Our Wilson-centric approach thus necessitates distinguishing between ordinary and projective representations, which correspond to different elements of the second cohomology group – they correspond to different sets of available band topologies.

\(M_z\) and \(t_\perp\) exemplify bulk symmetries that rule out certain topologies. Yet, not all bulk symmetries are disabling – Chap. 6 showed how spatial-inversion symmetry can enable a \(Z\) topology that is detectable by bulk transport but undetectable on the surface; here we
introduced the notion of a $\mathbb{Z}$-type relative-winding of the Wilson ‘bands’. Another enabling story arised in Chap. 7, where discrete rotations are combined with time-reversal symmetry. This last case study highlighted that bent Wilson loops have utility in topological band theory, even where they are not associated with any polarization quantity.
References


[60] Princeton theses. Refer to Chapter on ‘Spin-orbit-free topological insulators without time-reversal symmetry’.


[76] Refer to chapter on “hourglass dirac fermions and the crystalline spin hall effect”.


