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Chapter 4

The space group classification of topological band insulators

The theoretical prediction and experimental realization of the $\mathbb{Z}_2$-invariant topological band insulator (TBI) provided for a crucial boost in the revival of prominent interest in topological aspects of condensed matter systems and topological band theory in particular. As discussed in the introductory Chapters, these advancements found their foundation in the connection of the two a priori unrelated concepts of symmetry and topology, culminating in the construction of the tenfold periodic table. The role of the crystal lattice in this classification is to provide a unit cell in the momentum space, the Brillouin zone (BZ), topologically equivalent to the $d$-dimensional torus, over which the electronic Bloch wavefunctions are defined. The tenfold classification then follows by assuming that all the unitary symmetries of the corresponding Bloch Hamiltonian have been exhausted, rendering time reversal symmetry and particle hole symmetry as the only remaining anti-unitary symmetries due to Wigner’s theorem.

In three spatial dimensions (3D), however, by considering a $\mathbb{Z}_2$ TBI as a stack of two-dimensional (2D) ones, thus assuming a layered 3D lattice, additional three “weak” invariants associated with the discrete translation symmetry have been found [39]. Similarly, it has been realized that topological states protected just by inversion, can exist in 3D [38, 118, 119, 120, 121, 122]. Moreover, we demonstrated in the previous Chapter the existence of dislocation susceptible states that are protected by both TRS and the lattice $C_4$ rotational symmetry. Nonetheless, the generic role of the space group symmetries in the physics of topological states has remained elusive, in spite of these explicit
indicators.

In this Chapter, we bridge this gap and provide for the complete classification of TBIs protected not only by TRS, but also by space group lattice symmetries. Using this general formulation, that naturally incorporates the crystalline symmetries, we then identify three general classes of $\mathbb{Z}_2$ topological insulating states: (a) $\Gamma$ states robust against general time-reversal invariant perturbations; (b) Translationally-active states protected from elastic scattering, but susceptible to topological crystalline disorder; (c) Valley or crystalline topological insulators sensitive to the effects of non-topological and crystalline disorder. These three classes give in turn rise to 18 different two-dimensional, and, at least 70 three-dimensional TBIs, opening up a route for the systematic search for new types of TBIs.

4.1 Classification scheme and general principles

As a starting point, we depart from the construction by Fu and Kane [37, 38, 123] to compute the $\mathbb{Z}_2$ invariant in terms of the matrix of overlaps

$$w_{mn} = \langle u_m(-k)|\vartheta|u_n(k)\rangle,$$

(4.1)

where $\vartheta$ is the time-reversal operator and $|u_n(k)\rangle$ is the n-th occupied Bloch wavefunction. The quantities of central significance are

$$\delta_i = \sqrt{\det[w(\Gamma_i)]} \text{Pf}[w(\Gamma_i)],$$

(4.2)

evaluated at the points $\Gamma_i$ in the BZ where the Hamiltonian commutes with the time-reversal operator. Since the matrix $w$ is antisymmetric at the points $\Gamma_i$, the Pfaffian is well-defined at these points and $\det[w(\Gamma_i)] = (\text{Pf}[w(\Gamma_i)])^2$. The topological $\mathbb{Z}_2$ invariant, $\nu$, is then given by

$$( -1 )^\nu = \prod_{\Gamma_i} \delta_i,$$

and its non-triviality implies a topological obstruction for defining the wavefunctions through the entire BZ with an even number of band inversions. Heuristically, the above definition is thus yet another characterization of the fact that the mathematical vector bundle structure of a $\mathbb{Z}_2$ topological insulator features an odd number of non-trivial local transition maps, patching the wavefunctions globally in a topologically distinct manner over the Brillouin zone [25]. Notice also that the evaluation of the topological invariant in terms of the signs of the Pfaffian does not depend on the dimensionality but only on the fact that the Hamiltonian possesses TRS.
As a next step, the generality of Eq. (4.1) in conjunction with its momentum dependence can directly be exploited to signify the natural role of the underlying crystal symmetries. First, notice that the set of $\Gamma_i$ points at which the Hamiltonian commutes with the time-reversal operator is in fact fixed by the space group of the lattice, see Table 4.1. Second, it is evident that we may choose the overall phase of the Bloch wavefunctions so that a unique phase, which we dub the “$\Gamma$” phase, has $\delta_\Gamma = -1$ at the $\Gamma$-point in the BZ and $\delta_i = 1$ at all the other high symmetry points. The crucial observation then pertains to the fact that the distribution of signs of the Pfaffian, $\delta_i$, at the points $\Gamma_i$, and not only their product, resultantly encodes for additional topological structure. To show this, we first consider how the matrix of overlaps transforms under a lattice symmetry operation represented by a unitary operator $U$

$$w_{mn}(k) = \langle u_m(-k)|\vartheta|u_n(k)\rangle = \langle u_m(-Uk)|U\vartheta U^\dagger|u_n(Uk)\rangle = w_{mn}(Uk).$$  (4.3)

As a consequence, when some of these high symmetry points are related by a point-group symmetry of the lattice, their signs of the Pfaffian have to be equal. Therefore, it is sufficient to consider a subset, $\Gamma_a$, of representative, inequivalent high symmetry points that are also not related by any symmetry. This leads to the following rule that allows for determination of all the topological phases given the space group and the corresponding high symmetry points, $\Gamma_i$: each phase is obtained by selecting a single representative high-symmetry point $\Gamma_a$ and setting $\delta_\Gamma = -1$, which automatically sets $\delta_b = -1$ at all the high-symmetry points $\Gamma_b$ related by point group symmetry to $\Gamma_a$. Such phases are separated by a topological quantum phase transition that involves a bulk bandgap closing which then changes the values of $\delta_i$’s.

This simple classification principle can be illustrated by an elementary 2D example. We start with the $\Gamma$ phase on a square lattice, $\delta_\Gamma = -1$, and $\delta_X = \delta_Y = \delta_M = 1$ where $X$, $Y$, and $M$ are the time-reversal invariant (TRI) momenta in the BZ. By applying our rule, we immediately see that, besides the $\Gamma$ phase, we obtain an “$M$” phase with $\delta_M = -1$, and $\delta_X = \delta_Y = 1$ (Table 4.1). This phase is disconnected from the $\Gamma$ phase through a topological quantum phase transition with the band gap closing at the $X$ and $Y$ points and pertains to the “translationally-active” phase encountered in the previous Chapter. Recall that this phase is also protected by TRS, but exhibits, in contrast to the $\Gamma$ phase, susceptibility to dislocations. Furthermore, since the $X$ and the $Y$ points are related by a $C_4$ rotation, there can exist a phase with $\delta_X = \delta_Y = -1$, and $\delta_\Gamma = \delta_M = 1$. The product of the $\delta_i$’s at all TRI momenta then yields a trivial $Z_2$ invariant, $\nu = 0$. However, in this
Table 4.1: Table of the topological phases in two dimensions. For each of the lattice structures, the corresponding point-group (PG) symmetry and the relevant wallpaper group (WpG), i.e. space group, are given. The corners of the square and rectangle are denoted by M, whereas in the triangular Bravais structure they are indicated by K. Additionally, the centers of the edges are denoted by X and Y in both the square and rectangular case and by M in the other lattices [124]. The resulting phases are characterized by the distribution of $\delta_i$ at the $\Gamma_i$ points consistent with the WpG symmetry. Phases cluster in Bravais lattices, with the hexagonal structure being the only exception. In this case the WpGs containing six-fold and three-fold rotational symmetries relate the high symmetry points in different ways. As a result, the Hamiltonian does not commute with the time-reversal operator at the K points in the latter case. The obtained phases are ultimately protected by TRS (whenever $\nu = 1$), WpG symmetry, or both, and are accordingly indexed. The index (last column) describes the part of wallpaper group that leaves the subset $\Gamma_i$ having $\delta_i = -1$ invariant, while the additional label 'T' denotes TRS protection. In the column denoted “Phase” we introduce a convenient but imprecise shorthand notation.
case the $C_4$ rotational symmetry protects this phase, since it pins the band inversions at
the $X$ and $Y$ points, and therefore represents a “valley” or “crystalline” [119] insulator – a
phase trivial tenfold way-wise but protected by the lattice symmetries. Correspondingly,
this new phase, which we dub the “X-Y” phase, can similarly be realized in an extension
of the $M$-$B$ model for a quantum spin Hall insulator when next-nearest neighbor hopping
terms are incorporated, as shown in Fig. 4.1. Moreover, in accordance with the results
of the previous Chapter, such a phase also responds non-trivially to dislocations and
can therefore analogously be distinguished from the other phases due to the vectorial
entity of the Burgers vector, see Appendix 4.B. When the $C_4$ rotational symmetry is
reduced to $C_2$, the $X$ and $Y$ points are no longer related by symmetry, and therefore the
symmetry constraint on $\delta_X$ and $\delta_Y$ is no longer present. We then expect the X-Y phase
to be unstable, and to yield instead non-trivial phases with $\delta_X = -1$ or $\delta_Y = -1$, and
$\delta_i = 1$ at all other TRI momenta. Our calculations indeed confirm this within the M-B
tight-binding model. In general, an even number of TRI momenta related by symmetry
thus yields a valley or crystalline phase, protected by crystal symmetry while having $\nu = 0$, whereas in absence of this symmetry such a configuration renders a trivial phase.

Let us now elaborate on the role of the space group of the underlying lattice in this
classification, since this symmetry group defines the relation between the high symmetry
points. The difference in phases found on rectangular and rhombic lattices serves as
a clear illustration. Both these lattices have $D_2$ point-group symmetry, but different
wallpaper groups (space groups in 2D). The rhombic case has two inequivalent TRI
momenta related by a point group symmetry and hence a valley phase, see Table 4.1.
On the other hand, in the rectangular case all $D_2$ symmetry operations map any TRI
momentum to its equivalent, thus no crystalline phase is possible. From Table 4.1 it is
seen that in 2D the phases, as related to space groups, cluster in Bravais lattice classes,
with one exception: the hexagonal lattice. We will see that this clustering is less generic
in 3D. In turn, the primitive Bravais hexagonal (triangular) lattice ($p6mm$) is invariant
under the $C_6$ rotational symmetry around a lattice site, as opposed to the non-primitive
hexagonal lattice ($p3m1$) realized in graphene. Based on our rule, we conclude that in
the latter case only the $\Gamma$ phase is possible, which is in fact realized in the Kane-Mele
model [31, 32]. In contrast, on the former lattice (triangular), the points $K_+$ and $K_-$
are related by a $C_6$ symmetry and thus each of these points becomes TRI. The number
of TRI momenta is henceforth increased, ultimately yielding a possibility of additional
translationally-active and valley phases, as shown in Table 4.1 and Appendix 4.A.
Figure 4.1: Phase diagram of the extended $M - B$ tight-binding model. As function of the model parameters $M/B$ and $z = \tilde{B}/B$, where $B$ ($\tilde{B}$) is the (next) nearest-neighbor hopping parameter and $M$ the difference in on-site energies (Appendix 4.A), the different distributions of $\delta_i$ are obtained with the corresponding phases enlisted in Table 4.1. Furthermore, the spectra of edge states per spin component are displayed for the non-trivial phases, demonstrating that the valley X-Y phase exhibits a pair of Kramers pairs of metallic edge states. The real space localization of these edge states is also presented, where the radii of the circles represent the magnitude of the wave function and the colors indicate the phases as shown on the left.
The above rule allows us to completely classify and index the topological phases as conveyed by the last entry in Table 4.1. The set of BZ high-symmetry points $\Gamma_i$ at which there is band inversion, i.e., $\delta_{\Gamma_i} = -1$, is invariant under the operations of a subgroup of the lattice space group. This symmetry subgroup therefore protects, and labels, the topological phase. The other element in this indexing is the protection by TRS (T), existing when the $\mathbb{Z}_2$ invariant $\nu = 1$, giving, for instance $T - p4mm$ as the $\Gamma$ phase on the square lattice. When the protecting symmetries coincide between phases, we explicitly label $\Gamma_i$ (lower index), as, e.g., for $T - p2m_X$, $T - p2m_Y$ and $T - p2m_M$ phases on the rectangular lattice. This leads to the list of topological phases in 2D presented in Table 4.1 conveying 18 distinct topological phases. As our general result, we thus obtain two additional broad classes of topological states protected by TRS or crystalline symmetries, besides the class of states robust against general TRS perturbations ($\Gamma$-states): translationally-active states protected both by TRS and lattice symmetry, responding to dislocations, and valley insulators which are tenfold-way-wise trivial but protected by space group symmetry and also susceptible to dislocations.
<table>
<thead>
<tr>
<th>Bravais Lattice</th>
<th>PGS</th>
<th>SG</th>
<th>$\Gamma_i$</th>
<th>$\delta_i$</th>
<th>Index (Phase)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primitive Cubic</td>
<td>$O_h$</td>
<td>$pm\bar{3}m$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$pm\bar{3}n$</td>
<td></td>
<td>(-1,1,1,1)</td>
<td>$T-pm\bar{3}m$ ($\Gamma$)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$pm\bar{3}m$</td>
<td>(1,-1,1,1)</td>
<td>$T-p3(4)_R$ ($R$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$pm\bar{3}n$</td>
<td>(1,1,-1,1)</td>
<td>$T-p3(4)_X$ ($XYZ$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$(1,1,1,-1)$</td>
<td>$T-p3(4)_M$ ($MX'Y'$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$C_{6v}$</td>
<td>$p6mm$</td>
<td>$(\Gamma,M,A,L,K,H)$</td>
<td>(-1,1,1,1,1,1)</td>
<td>$T-p6mm$ ($\Gamma$)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$p6cc$</td>
<td>(1,-1,1,1,1,1)</td>
<td>$T-p6m$ ($M$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$p6_3cm$</td>
<td>(1,1,1,1,1,1)</td>
<td>$T-p6m_A$ ($A$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$p6_3mc$</td>
<td>(-1,1,1,1,1,-1)</td>
<td>$T-p6L$ ($L$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$-p6_3$</td>
<td>(1,1,1,1,1,1)</td>
<td>$T-p6_{6H}$ ($MH$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$-p6_3$</td>
<td>(1,1,1,1,-1,-1)</td>
<td>$T-p6_{6K}$ ($KA$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$-p6_3$</td>
<td>(1,1,1,1,1,1)</td>
<td>$p6K$ ($K$-valley)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$-p6_3$</td>
<td>(1,1,1,1,1,1)</td>
<td>$p6H$ ($H$-valley)</td>
<td></td>
</tr>
<tr>
<td>Face Centered Cubic</td>
<td>$O_h$</td>
<td>$f\bar{m}3m$</td>
<td></td>
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<td></td>
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<tr>
<td></td>
<td></td>
<td>$f\bar{m}3c$</td>
<td>(1,-1,1,1,1,1)</td>
<td>$T-f\bar{m}3m$ ($\Gamma$)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>$f\bar{m}3c$</td>
<td>(-1,1,1,1,1,1)</td>
<td>$T-f3(4)$ ($X$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$f\bar{m}3c$</td>
<td>(1,1,1,1,1,1)</td>
<td>$f\bar{3}U$ ($U$-valley)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$f\bar{m}3c$</td>
<td>(1,1,1,1,1,1)</td>
<td>$f\bar{3}W$ ($W$-valley)</td>
<td></td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>$D_{3d}$</td>
<td>$r\bar{3}m$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$r\bar{3}c$</td>
<td>(1,-1,1,1,1,1,1)</td>
<td>$T-r\bar{3}m$ ($\Gamma$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$r\bar{3}c$</td>
<td>(1,-1,1,1,1,1,1)</td>
<td>$T-r\bar{3}_L$ ($L$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$r\bar{3}c$</td>
<td>(1,1,-1,1,1,1,1)</td>
<td>$T-r\bar{3}_F$ ($F$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$r\bar{3}c$</td>
<td>(1,1,1,-1,1,1,1)</td>
<td>$T-r\bar{3}_Z$ ($Z$)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$r\bar{3}c$</td>
<td>(1,1,1,1,-1,1,1)</td>
<td>$r\bar{3}P$ ($P$-valley)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>$r\bar{3}c$</td>
<td>(1,1,1,1,1,-1,1)</td>
<td>$r\bar{3}K$ ($K$-valley)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>$r\bar{3}c$</td>
<td>(1,1,1,1,1,1,1)</td>
<td>$r\bar{3}B$ ($B$-valley)</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.2: Topological phases anticipated in 3D for some specific point group (PG) symmetries. Bravais lattices with same PG symmetries have different space groups (SG). We point out that, in contrast to the 2D case, the phases do not cluster in Bravais lattice structures. For example, the fourfold rotational symmetry crucial for the $f\bar{4}3_U$ and $f\bar{4}3_W$ phases is not contained in every space group associated with the face centered cubic lattice. As $\delta_i$’s attain the same value at the points $\Gamma_i$ related by lattice symmetry or a reciprocal lattice vector, only one representative is given from each set of such points. We note that the rhombohedral $T-r\bar{3}_L$ phase is observed in Bi$_x$Sb$_{1-x}$ [42, 125], while the $T-r\bar{3}_m$ phase is found in Bi$_2$Se$_3$ [43] and Bi$_2$Te$_3$[44]. Moreover, the $f\bar{m}3m$ – $f\bar{3}(4)$ phase has recently been observed in Pb-doped SnTe [126, 127].
4.1 Classification scheme and general principles

4.1.1 Three spatial dimensions

Our procedure can be applied in the same way in 3D, albeit becoming more involved given the 230 space groups and the large number of high-symmetry points. We find at least 70 different phases. Here we will illustrate matters for a number of simple crystal structures (Table 4.2) which include those of TBIs that are of present empirical relevance [42, 43, 44, 125]. In particular, consider the primitive cubic lattice (Table 4.2) with the familiar eight TRI points (Fig. 4.2A). Crucially, the points \((X, Y, Z)\) are related by a three-fold rotation, as well as the points \((X', Y', Z')\). Consequently, we obtain four TRS protected phases. We notice that this is quite different from the indexing procedure introduced by Moore and Balents [39]. For instance, our \(T - p\bar{3}m\) \((\Gamma)\) and \(T - p3(4)_R\) \((R)\) phases correspond with their \((1;0,0,0)\) and \((1;1,1,1)\) indices, respectively. Their latter two indices would, however, also correspond with the \(T - p3(4)_M\) and \(T - p3(4)_X\) phases. The other possibilities in their classification are either coincident with our four TBIs, or represent a 3D phase not protected by crystal symmetries due to implicit dimensional reduction (e.g. layered 3D lattice); see Figs. 4.2A,B.

The power of the space group classification becomes further manifest for non-cubic lattices. Consider the 3D hexagonal lattice which consists of two hexagonal layers with the wallpaper group \(p6mm\) stacked on top of each other. The TRI momenta comprise two copies of the ones on the 2D hexagonal lattice, separated by a perpendicular translation. Accordingly, the phases can easily be obtained by considering the \(k_z = 0\) plane (Table 4.1), which contains the \(\Gamma, M\) and \(K\) points, and those of the other translated plane associated with the points \(A, L\) and \(H\), respectively (Table 4.2). Consequently, there are eight TRS protected phases resulting from the combinations of a TRS protected phase in one plane and a trivial or a valley configuration in the other plane. Additionally, there are two valley phases which are configurations with one plane featuring a valley phase and the other a trivial configuration. Notice that a potential double valley phase with a valley phase in each of the planes is not protected by a 3D crystal symmetry and is therefore trivial. We again point out in this regard that the truly 3D crystalline phase is determined by a three-dimensional point group, i.e., the one whose action cannot be reduced to the 2D case.
Figure 4.2: Illustration of the role of lattice symmetries in the classification of topological states. (A) The eight TRI momenta in the Brillouin zone of the primitive cubic lattice. When only TRS is considered the sign of any quadruple of $\delta_i$'s within a plane connecting them can be changed, leaving their product the same. As a result one obtains, in addition to the 'strong' invariant, three weak invariants corresponding to the orthogonal planes. (B) The constraints on the $\delta_i$'s arising from the lattice symmetries. The high symmetry axes $\Delta$, $\Lambda$ and $\Sigma$ represent axes of four-, three- and two-fold rotations, respectively; these transform the TRI points in the colored planes into each other, and thus constrain the corresponding $\delta_i$'s to be equal. (C) The Brillouin zone of the face centered cubic lattice with high symmetry points and a mirror plane that projects onto the $\bar{\Gamma} - \bar{X} - \bar{\Gamma}$ line in the $(001)$ plane. The $W$-valley phase features Dirac cones along $\bar{\Gamma} - \bar{M} - \bar{\Gamma}$ and $\bar{\Gamma} - \bar{S} - \bar{\Gamma}$ lines, but not along $\bar{\Gamma} - \bar{X} - \bar{\Gamma}$ lines.
4.2 Topological signatures in the Greens function structure

As an intriguing sidestep, we remark that in the explicit context of the above simple lattice regularized Dirac Hamiltonians, the $\mathbb{Z}_2$ topological order can be characterized from a complementary point of view, that reflects the fundamental bulk-boundary correspondence and in turn signifies the general space group classification. Specifically, it turns out that the local in-gap Green’s functions $G_0(\varepsilon, k_\parallel, r_\perp = 0)$, with $r_\perp$ the position perpendicular to a codimension-1 or -2 surface, only attains zeros in the topological regime. These zeros are a direct consequence of the fact that the systems features a band inversion and thus characterize the non-trivial $\mathbb{Z}_2$ order. Moreover, by taking projections of the Green’s function onto different codimension-1 surfaces, one can then readily deduce the bulk TRI momentum at which the band inversion occurs, pertaining directly to the $\delta_i$ configuration of the space group classification.

To make this concrete, we revert to the models of the form of Equations (2.7) and (2.8),

$$H_0 = d_\mu(k) \gamma^\mu,$$

(4.4)

where $\Gamma^\mu$ are the $4 \times 4$ Dirac matrices with the $\sigma$ and $\tau$ Pauli matrices acting in the spin and orbital space, respectively, and $\mu = 0, 1, 2, 3$. Specifically, we choose $\gamma^0 = \sigma_0 \otimes \tau_3$ and $\gamma^i = \sigma_i \otimes \tau_1$. Recall, that time reversal symmetry (TRS) then implies that $d_0(k)$ must be an even and $d_i(k)$ must be an odd function of momentum. Focusing on the cases that $d_0(k) = M - 2B \sum_i (1 - \cos(k_i))$ and $d_i(k) = \sin(k_i)$, we then retrieve the familiar $M - B$ models in two and three spatial dimensions.

As a next step, consider a codimension-1 surface, having only one perpendicular direction $r_\perp = 0$. The corresponding simple real frequency Green’s function in the gap,

$$G_0(\omega, k) = \frac{1}{\omega - d_\mu(k) \gamma^\mu} = \frac{\omega \mathbf{1}_4 + d_\mu(k) \gamma^\mu}{\omega^2 - |d(k)|^2},$$

(4.5)

is then readily integrated over the associated perpendicular momentum. Moreover, the according result can subsequently be decomposed in terms of

$$g_\mu(\varepsilon, k_\parallel) = \int \frac{dk_\perp}{2\pi} \frac{d_\mu(k_\parallel, k_\perp)}{\varepsilon^2 - |d(k_\parallel, k_\perp)|^2},$$

(4.6)

and

$$g(\varepsilon, k_\parallel) = \int \frac{dk_\perp}{2\pi} \frac{\varepsilon}{\varepsilon^2 - |d(k_\parallel, k_\perp)|^2},$$

(4.7)
Figure 4.3: The flow of the poles of Eq. (4.9) as function of $M/B$. The two negative residue poles are indicated with a dot, whereas the stars mark the poles having a positive residue. In the trivial system, two poles with either positive or negative residue are located inside the red unit circle. For $M/B = 0,4$ there are two poles with opposite residue located on the unit circle, signaling the transition. The topological phase is characterized by two poles of opposite residue in the unit circle. Finally, the solid lines illustrate the curves of the poles for increasing $M/B$.

so that $G_0(\epsilon, k_\parallel, r_\perp = 0) = g(\epsilon, k_\parallel)1 + g_\mu(\epsilon, k_\parallel)\gamma^\mu$. This form shows that for any TRI point of the parallel momentum, for example $k_\parallel = 0$ or $k_\parallel = \pi$, the $g_\parallel$ components equate to zero. As a result, since the $g_\perp$ term also vanishes by virtue of the integrand being an odd function of $k_\perp$, we thus conclude that we only need to evaluate the projections $g_0$ and $g$ at TRI points. Moreover, it is noteworthy to observe that these considerations still hold in the presence of, for example, Rashba spin orbit coupling terms, that are odd functions of the momentum. In particular, as such Rashba terms remove the particle hole symmetry of the original Hamiltonian and similar terms can be introduced to eliminate the inversion symmetry, the subsequent results can therefore also be verified in the absence of any other symmetry but time reversal symmetry.

Let us now show that the eigenvalues of the in-gap Green’s functions $G_0(\epsilon, k_\parallel, r_\perp = 0)$ only comprise zeros in the topological regime. As a first step, we note that the denominator in the integrand, $\epsilon^2 - |d|^2$, is always negative. In the trivial phase $d_0(k)$ does not change sign throughout the Brillouin zone, implying that $g_0(\epsilon)$ does not change sign. Additionally, since $\epsilon < |d_0(k)|$, we furthermore deduce that $g(\epsilon) + |g_0(\epsilon)| > 0$ and $g(\epsilon) - |g_0(\epsilon)| < 0$. Hence, it is evident that the boundary Green’s function
shows that the residues of the two zeroes \( f \) with \( G \). We already infer that the regime \( 0 < \hat{M} < 4B \) is topologically distinct from \( \hat{M} < 0 \) and \( 4B < \hat{M} \). Focusing on the topological phase \( 0 < \hat{M} < 4B \), a straightforward evaluation shows that the residues of the two zeroes \( x_{0,\pm} = \frac{2B-\hat{M} \pm \sqrt{1-4BM+\hat{M}^2}}{2B \pm 1} \) located inside the unit circle cancel,

\[
\text{Res}(x_{0,+}) + \text{Res}(x_{0,-}) = 0, \tag{4.10}
\]

revealing that \( g_0(\varepsilon = 0) = 0 \) in the topological phase. Accordingly, when \( \hat{M} < 0 \) or \( 4B < \hat{M} \), representing the trivial regimes, the integral never equates to zero and together with the universal divergence of the both \( g(\varepsilon) \) and \( g_0(\varepsilon) \) at the band edges (see Appendix 4.C), we arrive at the generic description as shown in Fig. 4.4.

We thus observe that the number of zeros in the boundary Green’s function relates to the underlying topological characterization. That is, the odd number of crossings per spin branch of \( G_0(\varepsilon, k_\parallel, r_\perp = 0) \) with the zero eigenvalue axis is a topological property.
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Figure 4.4: The eigenvalues of the local Green’s function $G_0(\epsilon, k_\parallel = 0, r_\perp = 0)$ in the $M/B$ model corresponding with codimension-1 (left panel) and codimension-2 (right panel) surfaces. In the trivial system (dashed lines, $M/B = -1$) the eigenvalues $\lambda_\pm$ are nonzero. In the topological system (solid line, $M/B = 1$) the eigenvalues are zero for some in-gap energy and hence in-gap bound states on codimension-1 and codimension-2 impurities always exist. The dashed line $1/V_0$ in the left panel graphically marks these bound state solutions of codimension-1 impurities.

It reflects that in the non-trivial regime the system has an odd number of Kramers degenerate edge states on either side of the surface and hence may be regarded as a consequence of the bulk-boundary correspondence. In particular, the bulk TRS $\mathbb{Z}_2$ invariant for the above simple models is given by the product $\prod_{\Gamma_i} \xi_i$ of the parity $\gamma_0$ eigenvalues $\xi_i$ over the TRI points in the Brillouin zone [38] and the two relevant poles have the same residues but multiplied by the sign of the mass, i.e. the parity $\gamma_0$ eigenvalues. For that reason, only if the choice $k_S$ in the projected plane is associated with two masses of opposite sign, meaning that this cut features a band inversion, the poles cancel in the above integral rendering a zero eigenvalue. This is in direct accordance with the space group classification.

For example, the two dimensional variant of Equation (4.4) exhibits a $\Gamma (T-p4mm)$ phase for $0 < M/B < 4$ and a $M (T-p4)$ phase for $4 < M/B < 8$. From the above considerations we find that $\tilde{M}$ has to satisfy $0 < \tilde{M} < 4$ for $G_0(\epsilon, k_\parallel, r_\perp = 0)$ to develop zero eigenvalues. Taking subsequently projections along the $k_x$ and $k_y$ directions and using that $\tilde{M}(k_S) = M - 2B(1 - \cos(k_s))$, we thus conclude that in the $\Gamma$ phase the $k_S$ values exhibiting a zero eigenvalue correspond to projections of the inversion momentum $\Gamma_l = \Gamma$, whereas in the $M$ phase they are associated with a bulk inversion $\Gamma_l = M$. We stress that this analysis still holds if we add Rashba terms, or other TRS perturbation
4.2 Topological signatures in the Greens function structure

terms that are odd functions of momentum. Similarly, when we add the next nearest
neighbor term (Appendix 4.A) to the Hamiltonian and tune the system into the $X - Y$
($p4$) topological crystalline phase, the inversion momenta correspond with $\Gamma_I = X$ and
$\Gamma_I = Y$ as conveyed by Table (4.1). An identical calculation then shows that the pro-
jections along $k_x$ and $k_y$ feature indeed zero eigenvalues of $G_0(\epsilon, k_\parallel, r_\perp = 0)$ for both
$k_S = 0$ and $k_S = \pi$. These principles are exemplified in the three dimensional instances
in the exact same fashion. Considering for example a $\Gamma (T - pm\overline{3}m)$ phase featuring an
inversion at $\Gamma_I = \Gamma$ for $0 < M/B < 4$, it is evident that $k_S$ corresponds with $(0, 0)$ in any
of the planes normal to the principle axes.

The above results on the structure of the eigenvalues of $G_0(\epsilon, k_\parallel, r_\perp = 0)$ in the
codimension-1 case can similarly be extended to codimension-2 surfaces (Fig. (4.4)).
Specifically, also in the latter instance the associated local in-gap Green’s function only
attains zeros if and only if the system is in the topological phase, as detailed in the
Appendix 4.C. Although, these zeros are no longer in direct correspondence with the
space group classification due to second integration procedure, this result does provide
for another experimental signature of the TRS induced $Z_2$ invariant in the context of
impurity bound states. Concretely, for an impurity defect that preserves translational
symmetry along the parallel directions $r_\parallel$, the defining eigenvalue equation determining
the existence of in-gap bound states is given by [132, 133]

$$\det [G_0(\epsilon, k_\parallel, r_\perp = 0)V_0 - 1] = 0,$$

where $V_0$ is the specific form of the impurity. As a result, considering an impurity of the
form

$$V(r) = V_0 \delta_{r_\perp = 0},$$

we observe that in the topological phase a codimension-1 or -2 impurity will always
result in a in-gap bound state, whereas in the trivial regime this depends on the details
[133]. Accordingly, one could imagine a two-dimensional insulator, where at one iso-
lated point a tunable gate voltage is applied, serving as the impurity potential $V$. Then
using tunneling spectroscopy, the possible bound states around this impurity can read-
ily be identified. However, upon increasing the impurity potential $V$, the energies of the
bound states will shift and for a trivial insulator one can make the bound states disappear
into one of the bands for a sufficiently strong potential. In contrast, for a topological in-
sulator the above shows that for all $V$ there will always be two in-gap bound states (Fig.
4.5), providing for a clear indication of the non-trivial $Z_2$ invariant.
Figure 4.5: Typical energy of impurity bound states in a two-dimensional insulator as a function of impurity strength $V$. Here, we discern between the topological regime (solid lines, $M/B = 1$) and the trivial regime (dashed line, $M/B = -1$). For strong $V$, bound states in the trivial phase have disappeared in the conduction band, whereas the bound states in the topological phase remain.

4.3 The space group classification as an experimental guide

Let us now return to the general classification scheme and discuss its relevance in the scenery of experimentally viable TBIs. A lot of observed TBIs, including the second generation Bi-based materials Bi$_2$Se$_3$ [43] and Bi$_2$Te$_3$[44], are of the $\Gamma$ kind. Nonetheless, the compound which initiated the 3D pursuit, Bi$_x$Sb$_{1-x}$, is a non-$\Gamma$ TBI, characterized by $r\bar{3}m - T - r\bar{3}L$ [42, 125]. Similarly, the theoretically predicted rock-salt actinides [134] are associated with the translationally-active class and exemplify a $fm\bar{3}m - T - f\bar{3}L$ phase. Furthermore, the predicted valley or crystalline class found recent experimental verification in the form of Pb-doped SnTe [126, 127]. Most interestingly, this latter system has the exact same space group, $fm\bar{3}m$, as the actinides. Hence, we are directly confronted with the effective working of the space group classification. Given the specific crystal symmetry group, one directly obtains the possible phases as conveyed by Table (4.2).

As a final demonstration of the general principle, let us consider the latter valley phase, indexed by $fm\bar{3}m - f\bar{3}L$, in more detail. This system features mirror planes in the momentum space formed by the $\Gamma$ and any two of the $L$ points, which thereby relate the remaining two $L$ points by symmetry. As a result, a mirror-symmetric crystal cut along $\tilde{\Gamma} - \tilde{X} - \tilde{\Gamma}$ line in the (001) surface exhibits a pair of Dirac cones (a double
Dirac cone) which is therefore also protected by the same symmetry [120]. Notice that in addition we predict valley phases at the $W$ and the $U$ points in the Brillouin zone protected by both the four-fold and the three-fold rotational symmetries, labelled by $fm\bar{3}m - f43w$ and $fm\bar{3}m - f43u$, respectively. The $W$-phase originates from six inequivalent symmetry-related $W$-points in the BZ where a band inversion gives rise to a valley phase. In addition, in the same phase, the $(001)$ surface features Dirac cones for the cut along $\bar{\Gamma} - \bar{M} - \bar{\Gamma}$ and $\bar{\Gamma} - \tilde{S} - \bar{\Gamma}$ lines, but not along $\bar{\Gamma} - \bar{X} - \bar{\Gamma}$ direction, as it is the case in the $fm\bar{3}m - f3(4)$ phase, see Fig.4.2(C). Therefore, the detection of the Dirac cones in the $\bar{\Gamma} - \bar{M} - \bar{\Gamma}$ and $\bar{\Gamma} - \tilde{S} - \bar{\Gamma}$ directions in ARPES experiments would be a clear signature of this valley phase.

4.4 Conclusions

In conclusion, we provided the space group classification of topological band insulators in both in two and three spatial dimensions. As a main result, this classification scheme identifies two additional broad classes of topological phases, besides the TRS protected $\Gamma$ states: translationally-active phases, protected by both TRS and crystal symmetries, but susceptible to topological crystalline disorder, and valley phases solely protected by the space group symmetry, and therefore susceptible to both elastic and topological crystalline disorder. These classes correspond directly to the results of the previous Chapter and can similarly be probed by dislocations. Furthermore, a non-trivial characterization of the bulk also leads to a distinct zeros in the Green’s function structure associated with codimension-1 surfaces, which in fact is a consequence of the bulk-boundary correspondence. The resulting pattern of projected zeros resultantly indicates the space group classification from a complementary perspective. Finally, our complete classification scheme based on the full 2D and 3D space groups has as most important experimental consequence that it demonstrates the potential existence of at least seventy distinct topological phases of insulating matter and we anticipate that this will be a valuable guide in the future exploration of this landscape.
4.A Verification within M-B model setting

The above general notions can directly be corroborated within the specific setting of the previous Chapters. Let us therefore for concreteness illustrate the general principles in this context. In particular, it is straightforward to generalize the $M-B$ model eq. (3.41) to the five Bravais structures in two spatial dimensions. The connection to the above characterization is then readily achieved by noting that the Pfaffian expression relates to the band-structure vector $d^\Gamma_i$ of Eq. (3.37) through

$$\delta_i = \text{sign}[d_3(\Gamma_i)].$$

In case of the square lattice, the $C_4$ rotation connects the $\delta_i$’s and thus dictates that the values at the $X$ and $Y$ points have to be the same. In addition to the $\Gamma$ phase and $M$ phase, the anticipated crystalline phase can then be established by incorporating a next nearest neighbor term with the parameters defined exactly as in the nearest neighbor case. Accordingly, we obtain

$$d(k) = \begin{pmatrix}
\sin(k_x) + \cos(k_x) \sin(k_y) \\
-\sin(k_y) - \sin(k_x) \cos(k_y) \\
M - 2B[2 - \cos(k_x) - \cos(k_y)] - 4\tilde{B}[1 - \cos(k_x) \cos(k_y)]
\end{pmatrix}.$$

The gap at the TRI momenta and hence the configuration of $\delta_i$ can be tuned as function of the parameters $\tilde{B}/B$ and $M/B$ resulting in the phase diagram shown in Fig. 4.1. Importantly, we find that the resulting valley phase features two pairs of edge states. Connecting to the intuitive skyrmion picture, it can similarly be shown that this phase exhibits two Skyrmions located at the $X$ and $Y$ points and that integration of the Skyrmion density accordingly yields a winding number that equates to two per spin.

As the next step, the rectangular model is obtained by making the magnitude of the hopping parameters anisotropic, which effectively reduces the fourfold rotational symmetry to a twofold symmetry, see also Appendix 4.B, Eq. (4.18). Consequently, the oppositely valued $\delta_i$’s can be located at any of the TRI momenta $\Gamma, M, X, Y$, and the corresponding phases can be distinguished by insertion of dislocations (Appendix 4.B). We find that by increasing the ratio $r$ of the hopping magnitudes in the $y$ and $x$ directions the valley phase is lost: the system either enters a trivial state, a translationally-active $X$ phase or a phase with $C = 2$ per spin not protected by either TRS or lattice symmetry. Namely, only the former two phases are realized when the ratio $r$ is large enough. The two edge modes per spin in the $X$-$Y$ valley phase are gapped out upon an infinitesimal breaking of $C_4$ symmetry, i.e. by $r > 1$. The phase diagram of the model for $r = 2$ is
shown in Fig. 4.10.

![Brillouin Zone Diagram](image)

Figure 4.6: The Brillouin zone of the primitive hexagonal (triangular) lattice and the phase diagram of the M-B tight-binding model on the same lattice. High-symmetry points in the Brillouin zone at which the Hamiltonian commutes with the time-reversal operator are indicated. Additionally, the Chern number per spin block ($C = C_{\uparrow} = -C_{\downarrow}$) is shown for each phase.

In case of a primitive hexagonal (triangular) lattice with the wallpaper group $p6mm$, the nearest neighbor hopping part of the Hamiltonian is described by

$$d(k) = \begin{pmatrix} \sin k_x + 2\sin(k_y/2)\cos(\pi/3)\cos(\sqrt{3}k_y/2) \\ -2\cos(k_y/2)\sin(\pi/3)\sin(\sqrt{3}k_y/2) \\ M - 2B[2 - \cos k_x - 2\cos(k_y^3/2)\cos(\sqrt{3}k_y)] \end{pmatrix}. \quad (4.14)$$

As for the other Bravais lattices, the sign of the Pfaffian at the $\Gamma_i$ points is given by $\delta_i = \text{sign}[d_3(\Gamma_i)]$ and we observe that due to the very presence of the lattice symmetry ($C_6$ in particular), $\delta_i$ is also well defined at the two inequivalent corners $K_+$ and $K_-$ of the Brillouin zone (Fig. 4.6). Additionally, the symmetry relates the centers of the edges $M$ and we thus expect the phases as indicated in the Table 4.1. The resulting Hamiltonian corresponding to the vector $d$ in (4.14) indeed exhibits the $\Gamma$ and the $K$ valley phase for $-2 < M/B < 6$ and $6 < M/B < 7$, respectively. The $M$ phase can also be captured by including the next nearest neighbor hopping term

$$\tilde{d}(k) = \begin{pmatrix} A\sin(\sqrt{3}k_y)\cos(\pi/6)\cos(\sqrt{3}k_y) \\ -A[\sin(\sqrt{3}k_y) - 2\cos(\sqrt{3}k_y)\sin(\pi/6)\sin(\sqrt{3}k_y)] \\ -2B[3 - \cos(\sqrt{3}k_y) - 2\cos(\sqrt{3}k_y)\cos(\sqrt{3}k_y)] \end{pmatrix}. \quad (4.15)$$

For strong enough next-nearest neighbor hopping, \( z = \frac{\tilde{B}}{B} > \frac{1}{8} \), the gap closes at the \( K \) points before closing at the \( M \) points for increasing \( M/B \) and as a result the system exhibits a \( \Gamma \) and \( M \) phase, see Figs. 4.6 and 4.7. We note that we need six inequivalent high symmetry points, marked in Fig. 4.6, to capture the three observed phases within the rule presented in the main text. In contrast, the symmetry relating \( K_+ \) and \( K_- \) can readily be broken by considering a non-primitive honeycomb lattice structure, realized in graphene, which then makes \( K_\pm \) related by TRS. The Hamiltonian does not commute with the time-reversal operator at these points, and therefore, these two points no longer belong to the set \( \Gamma_i \). As the \( M \) points are still related by symmetry, we expect only a \( \Gamma \) phase in this case. A prominent example is the Kane-Mele model [32] with the configuration of \( \delta_i \)'s explicitly calculated in Ref. [38] using a rhombic unit cell. Drawing this cell in the extended BZ we observe that this configuration indeed corresponds with a \( \Gamma \) phase in the usual Wigner-Seitz cell. Additionally, the result can also be understood from the Skyrmion picture. Due to inversion-asymmetry the gap closes at \( K_\pm \) points instead of closing at the TRI momenta [135, 136]. The spin sub-blocks exhibit merons at \( K_+ \) and \( K_- \) points which can be explicitly shown by rewriting the Pontryagin index as in Ref [137].

![Figure 4.7: The skyrmion lattices in the extended Brillouin zone for the three topological phases on the primitive hexagonal (triangular) lattice. The locus of the Skyrmions is colored in red. (A) The Skyrmion lattice for the \( \Gamma \) phases within the M-B model. (B) \( K \) valley phase within the same model. (C) When next nearest neighbor hopping, \( z = \frac{\tilde{B}}{B} \), is taken into account, the system can enter the \( M \) phase, which has the Skyrmions positioned at the \( M \) points.](image-url)
Finally, we consider the oblique and rhombic Bravais structures distinguished by the presence of mirror symmetry in the latter case. This symmetry is ultimately responsible for the existence of the valley phase on the rhombic lattice. Considering the rhombic lattice, it can be readily shown that

\[
\mathbf{d}(\mathbf{k}) = \begin{pmatrix}
A_1 \cos(\phi_1) \sin(\tilde{k}_x) \cos(\tilde{k}_y) + A_2 \sin(r_1 k_x) \\
-A_1 \sin(\phi_1) \sin(\tilde{k}_x) \cos(\tilde{k}_y) - A_3 \sin(r_2 k_y) \\
M - 4B[1 - \cos(\tilde{k}_x) \cos(\tilde{k}_y)] + 2\tilde{B}[\tau_1^{-1} + \tau_2^{-1} - \tau_1^{-1} \cos(r_1 k_x) - \tau_2^{-1} \cos(r_2 k_y)]
\end{pmatrix},
\]

where \( \tilde{k}_x = e_1 \cos(\phi_1) k_x, \tilde{k}_y = e_1 \sin(\phi_1) k_y, \) with \( \phi_1 \) being the polar angle of the vector \( \mathbf{e}_1, \) and \( e_1 = |\mathbf{e}_1|; \) see Fig. 4.8. Furthermore, \( A_i \) is the hopping between the \( s \) and the \( p \) orbitals along the vector \( \mathbf{e}_i, \) while \( B \) is the hopping between the two \( s \) orbitals along the vector \( \mathbf{e}_1, \) and the hopping between these orbitals along the vectors \( \mathbf{e}_{2,3} \) is \( B_{2,3} = \tilde{B}\tau_{2,3}^{-1}. \) Due to the mirror symmetry, the \( M_{-1} \) and \( M_1 \) points are connected and as a result the gap closes at these points for the same value of \( M/B. \) Consequently, tuning the gaps at the TRI momenta by varying the parameters of the model, the configurations of \( \delta_i \)'s and the corresponding phases shown in Table 1 in the main text are easily obtained. The oblique lattice can be then treated similarly. Denoting the different connections between neighbors as indicated in Fig. 4.9, we obtain

\[
\mathbf{d}(\mathbf{k}) = \begin{pmatrix}
A_1 \cos(\phi_1) \sin(\mathbf{e}_1 \cdot \mathbf{k}) + A_2 \cos(\phi_2) \sin(\mathbf{e}_2 \cdot \mathbf{k}) + A_3 \cos(\phi_3) \sin(\mathbf{e}_3 \cdot \mathbf{k}) + A_4 \cos(\phi_4) \sin(\mathbf{e}_4 \cdot \mathbf{k}) \\
-A_1 \sin(\phi_1) \sin(\mathbf{e}_1 \cdot \mathbf{k}) - A_2 \sin(\phi_2) \sin(\mathbf{e}_2 \cdot \mathbf{k}) - A_3 \sin(\phi_3) \sin(\mathbf{e}_3 \cdot \mathbf{k}) - A_4 \sin(\phi_4) \sin(\mathbf{e}_4 \cdot \mathbf{k}) \\
M - 2B[2 - \tau_1^{-1} \cos(\mathbf{e}_1 \cdot \mathbf{k}) - \tau_2^{-1} \cos(\mathbf{e}_2 \cdot \mathbf{k}) - \tau_3^{-1} \cos(\mathbf{e}_3 \cdot \mathbf{k}) - \tau_4^{-1} \cos(\mathbf{e}_4 \cdot \mathbf{k})]
\end{pmatrix},
\]

where the angles \( \phi_i, i = 1, \ldots, 4, \) are the polar angles of vectors \( \mathbf{e}_i. \) The \( s - p \) hopping along the vector \( \mathbf{e}_i \) is \( A_i, \) and the \( s - s \) hopping along the same vector is \( B_i = B\tau_i^{-1}. \)
Again, by varying the model parameters (consequently also the shape of the BZ), it is straightforward to realize the different phases which are also visualized by the presence of a Skyrmion at either of the indicated points. More interestingly, the analysis confirms yet again the significance of the symmetry group of the underlying crystal. Essentially, the only difference between the oblique and rhombic systems is the presence of the mirror symmetry. Therefore, the same \((1,1,-1,-1)\) configuration of \(\delta_i\)'s results in a valley phase with the Chern number equal two per spin block only when the mirror symmetry is present, i.e., only in the case of the rhombic lattice.

![Figure 4.9: The real space oblique lattice and its corresponding Brillouin zone. In contrast to the rhombic case, the TRI momenta are not related by a lattice symmetry. In this example, vectors \(e_1\) and \(e_2\) connect nearest-neighboring sites, while \(e_3\) and \(e_4\) connect next-nearest neighboring sites.](image)

### 4.B Probing the topologically non-trivial phases

As shown in the previous Chapter, a \(\pi\)-flux probes \(Z_2\) topological order through the binding of the zero modes, while the dislocations act as universal probes of the translationally-active topological states. Although the generality of the above argument already implies analogous responses in accordance with the general space group classification, let us here demonstrate that indeed the same results hold within the extended \(M-B\) tight-binding model. In particular, focussing on the rectangular lattice model and the square lattice valley phase this then allows for motivation of the unique status of the dislocation directionality as a probe that distinguishes translationally-active and crystalline topological phases at different high symmetry points in the BZ.
The \( M-B \) tight-binding model on a rectangular lattice assumes the form (3.36) in terms of the vector
\[
d(k) = \begin{pmatrix}
\sin(k_x) + \frac{\hat{A}}{\sqrt{1+\tau}} \cos(\varphi_r)[\sin(k_+) - \sin(k_-)] \\
-1/\tau \sin(rk_y) - \frac{\hat{A}}{\sqrt{1+\tau}} \sin(\varphi_r)[\sin(k_+) + \sin(k_-)] \\
M - 2B[2 - \cos(k_x) - 1/\tau \cos(rk_y)] - 2\hat{A}[2 - \cos(k_+) - \cos(k_-)]
\end{pmatrix},
\]
where \( r \) denotes the ratio of the lattice spacing in the \( y \) and the \( x \)-direction, \( \varphi_r = \arctan(r) \), \( \tau = A_x/A_y = B_x/B_y \), and \( k_{\pm} = \pm k_x + rk_y \). In the remainder we conveniently fix \( r = \tau = 2 \) and \( \hat{A} = 1 \). The resulting phase diagram is presented in Fig. 4.10.

![Phase diagram of the extended M-B model on the rectangular lattice in Eq. (4.18) for \( r = \tau = 2 \) and \( \hat{A} = 1 \). The non-trivial phases include the \( \Gamma \), \( M \) and a \( X \) phases. Additionally, the Chern character \( C \) per spin, \( C = C_\uparrow = -C_\downarrow \), is indicated.](image)

Considering first only nearest neighbor hopping, the non-trivial phases on both the square and rectangular lattices include the \( \Gamma \) and \( M \) phases. Accordingly, we find that the \( M \) phase gives rise to a dislocation zero-mode, whereas a \( \pi \) flux results in a zero-mode in both the \( \Gamma \) and the \( M \) phase (Fig. (4.11)). The dislocation zero mode hybridizes with the low-energy edge states in a finite system. Separating these states by introducing weak disorder via a random chemical potential, we confirm that the edge state indeed pertains to the finite momentum \( k = \pi \).

The next nearest neighbor hopping, as already shown, realizes the valley phase on the square lattice (Fig. (4.1)). As anticipated, introduction of a magnetic \( \pi \) flux results in a double Kramers pairs of zero modes in the system. More interestingly, the
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Figure 4.11: Effect of introducing a $\pi$ flux or dislocations in the $\Gamma$ and $M$ phase of the square lattice model. The top row shows two zero-modes bound to $\pi$-anti-$\pi$ flux pair (periodic boundary conditions) appearing in the spectrum in case of the $\Gamma$ phase and the real space localization of these modes. For convenience we only consider one spin component. The bottom row shows the effect of a dislocation-anti-dislocation pair (periodic boundary conditions) with Burgers vector $b = e_y$ in the $M$ phase. The lattices contain $33 \times 33$ unit cells.

bulk-boundary correspondence and the directional character of a dislocation result in the possibility of discriminating between the two valley points. Namely, a dislocation with Burgers vector $b$ along the $\hat{x}$ or $\hat{y}$ direction binds only a single pair of zero-energy modes. Analysis of the edge state hybridized with the dislocation zero-mode then confirms that the dislocation indeed corresponds with the valley at the momentum parallel to the direction of the Burgers vector (Fig. 4.12).

When $r$ is increased (breaking square symmetry to rectangle), the Chern number per spin block may reduce to zero and insertion of a $\pi$-flux or a dislocation no longer results in a zero-mode in the system, confirming the intimate relation between the point group lattice symmetry and the valley phase. As the parameter $r$ is increased, another possibility is a topological phase transition to the $X$ phase which does not respect the fourfold symmetry and thus distinguishes the square from the rectangular lattice. This is reflected in the response of the system upon the insertion of dislocations. In addition
4.B Probing the topologically non-trivial phases

Figure 4.12: Probing the $X-Y$ valley phase, by considering one spin component of each Kramers pair. (A) Spectrum in presence of a $\pi$-flux and anti-$\pi$-flux in a periodic system. (B) Spectrum in case of a dislocation and anti-dislocation in a periodic system. (C) Real space localization of zero-mode resulting from a single dislocation with Burgers vector $b = e_y$. (D) The phase of the edge state hybridized with the dislocation zero mode displayed in (C), shows that it is a mode from the $Y$ point, $k = (0, \pi)$. Similarly, the dislocation zero-mode displayed in (F) hybridizes with edge state shown in (E), the phases of which indicate that this zero-energy state corresponds with the $X$ point, $k = (\pi, 0)$. Color-code is as in Fig. 4.1. The lattices contain $33 \times 33$ unit cells.

to the usual zero-energy modes resulting from a $\pi$-flux vortex, the spectrum shows a Kramers pair of zero-modes resulting from dislocations only if the Burgers vector $b$ has a component in the $x$ direction (Fig. 4.13).
Let us conclude by addressing the robustness of the zero-modes in the topological non-trivial regimes, which is related to the stability of the corresponding phase. To this end, we multiply all the model parameters by Gaussian variables of width $w = 10\%$ and also introduce Gaussian random chemical disorder, while preserving TRS. Moreover, we couple the spin-reversed sub-blocks by adding the familiar nearest neighbor Rashba spin-orbit coupling

$$H_R = i R_0 \frac{1}{2} \sum_{\mathbf{R}, \delta} \Psi^\dagger_{\mathbf{R}} [(\tau_0 + \tau_3) \otimes (\sigma \times \delta) \cdot \mathbf{e}_z] \Psi_{\mathbf{R} + \delta}$$ (4.19)

to the original Hamiltonian, which breaks the reflection symmetry $\varepsilon \rightarrow -\varepsilon$ about the plane. The results are displayed in Fig. 4.14. We find that finite Rashba spin orbit coupling, but not large enough to close the topological gap, preserves the real space localization of the mid gap modes. More importantly, we observe that the stability of the modes in the valley phase is significantly smaller than in the $Z_2$ non-trivial phases. We note that the latter phase has a smaller gap and hence would already require a weaker Rashba coupling to close the gap. However, one would expect the valley phase to be less stable independently of the gap size, as only the lattice symmetry accounts for its protection. To check this assertion, we also considered the valley phase in presence of a stronger next nearest neighbor hopping, which leads to an increase of the gap size. This analysis then confirms that the zero-modes in the valley phase are substantially less robust than those in the TRS protected phases. That is, the dis ordering terms close the
gap for smaller values in magnitude.

Figure 4.14: The averaged (over 130 disorder realizations) density of states (DOS) for various values of $M/B$, $z = \tilde{B}/B$ and $R = R_0/B$. Panels (A)-(B) and (D)-(E) correspond to the square lattice model, whereas panel (C) corresponds to the rectangular case. The midgap modes resulting from dislocations are present even for strong Rashba coupling and disorder, as demonstrated by (A) $R = 1.5$ in the $M$ phase, (B) $R = 0.5$ in the $X-Y$ valley phase and (C) $R = 1.5$ in the $X$-phase. Sufficiently strong Rashba coupling closes the topological gap, as shown for (D) $R = 2$ in the $M$ phase (a similar result is obtained for the $X$-phase) and (E) $R = 1$ in the $X-Y$ valley phase. Even for comparable values of the bulk gap, the valley phase is substantially less robust to the Rashba coupling than the TRS protected $M$ and $X$ phases.

4.C Topological signatures in the Greens function structure

In this Appendix, we provide some details regarding the evaluation of the Greens functions associated with codimension-1 and codimension-2 surfaces.

4.C.1 Details codimension-1 case

We have shown in the main text that $G_0(\varepsilon = 0, k_\parallel = k_S, r_\perp = 0) = 0$ only acquires zero eigenvalues in the topological regime. Here, we elaborate on the generic structure which results in the schematic representation as conveyed in Fig. 4.4. In particular, let us
address the behavior of $G_0$ close to the band edges. First, note that $g(\varepsilon)$ is a decreasing odd function in $\varepsilon$, and $g_0(\varepsilon)$ is an even function in $\varepsilon$. Close to the band edges, both $g(\varepsilon)$ and $g_0(\varepsilon)$ will always diverge as a square root, $g \sim 1/\sqrt{\delta \varepsilon}$. Whenever the gap is located at a $T$-symmetric point, where $d_i(\mathbf{k}) = 0$, the strengths of the divergences in $g(\varepsilon)$ and $g_0(\varepsilon)$ are equal. To prove we first consider the regime $m < \frac{1}{2}$ where the gap is located at $\mathbf{k} = 0$. We expand $|d(\mathbf{k}_\parallel = 0, k_\perp)|^2$ around that point,

$$|d(\mathbf{k}_\parallel = 0, k_\perp)|^2 = m^2 + (1 - 2m)k_\perp^2 + \ldots$$

The divergence of $g(\varepsilon)$ near the valence band edge can then be isolated by integrating over a small region $(-\alpha, \alpha)$ around the top of the valence band for small $\delta \varepsilon = \varepsilon + |m|$, 

$$g(\varepsilon = -|m| + \delta \varepsilon) \approx \int_{-\alpha}^{\alpha} \frac{dk_\perp}{2\pi} \frac{|m|}{2|m|\delta \varepsilon + (1 - 2m)k_\perp^2}$$

$$\approx \sqrt{\frac{|m|}{8(1 - 2m)\delta \varepsilon}} + O(\delta \varepsilon^0).$$

A similar argument applies to $g_0(\varepsilon)$ close to the valence band, as the magnitude of the gap $|d_0(\mathbf{k}_\parallel = 0, k_\perp = 0)| = |m|$. Therefore $g_0(\varepsilon)$ and $g(\varepsilon)$ have exactly the same divergent behavior close to the band edge. Hence, $g + |g_0|$ only diverges close to the valence band and $g - |g_0|$ diverges close to the conduction band. Note that this analysis is valid for $m < \frac{1}{2}$, when the band gap is at $\mathbf{k} = (0, 0)$, and for $m > \frac{15}{2}$, when the band gap is at $\mathbf{k} = (\pi, \pi)$. This implies that this cancellation of divergences is present in the trivial phase (in accordance with the notion that in this phase the eigenvalues do not change sign), but also for some region in the topological phase. In the latter case, the eigenvalue beaches of $G_0$ thus also diverge at either the valence or conduction band but do cross zero, in contrast to the trivial regime.

When $m > 1/2$ and $m < 15/2$, the gap is not located at a $T$-symmetric point but rather at $(0, k_G)$ or $(\pi, k_G)$. In this case, the gap satisfies $\Delta^2 = d_0(k_G)^2 + \sin^2 k_G > d_0(k_G)^2$. This last point is important, because then at any TRI point of $\mathbf{k}_\parallel$, the eigenvalues of $G_0(\varepsilon, k_\parallel^S)$ will both diverge to positive infinity at the valence band edge. To see this, we expand 

$$|d(\mathbf{k})|^2 = \Delta^2 + a(k_\perp - k_G)^2 + \ldots$$

so that the divergent parts close to the valence band edge of the Greens function terms
are
\[ g(\epsilon = -|\Delta| + \delta \epsilon) \sim \frac{|\Delta|}{\sqrt{8a|\Delta| \delta \epsilon}} \]
\[ g_0(\epsilon = -|\Delta| + \delta \epsilon) \sim -\frac{d_0(0, k_G)}{\sqrt{8a|\Delta| \delta \epsilon}}. \]

Because $|\Delta| > |d_0|$, we find that the divergences do not cancel and both eigenvalues of $G_0(\epsilon, k_\parallel)$ will diverge to positive infinity at the valence band edge. This means that at the conduction band edge, both diverge to negative infinity, therefore implying an energy at which $G_0(\epsilon)$ has zero eigenvalues.

4.C.2 Details codimension-2 case

In the case of a codimension-2 surface, there are two perpendicular directions $k_\perp = (k^x_\perp, k^y_\perp)$, and a similar decomposition as in the main text is given in terms of

\[ G_\mu(\epsilon, k_\parallel) = \int \frac{dk^x_\perp dk^y_\perp}{(2\pi)^2} \frac{d_\mu(k_\parallel, k_\perp)}{\epsilon^2 - |d(k_\parallel, k_\perp)|^2}, \]
\[ G(\epsilon, k_\parallel) = \int \frac{dk^x_\perp dk^y_\perp}{(2\pi)^2} \frac{\epsilon}{\epsilon^2 - |d(k_\parallel, k_\perp)|^2}, \]

for $\mu = 0, 1, 2, 3$. It is clear that for any of the perpendicular directions $G_\perp$ still equates to zero, as the integrand is odd. Also, for the trivial phase, it is straightforwardly seen that the eigenvalues of $G_0(\epsilon, k_\parallel, r_\perp = 0)$ are again nonzero throughout the gap. This is because the two-dimensional integral can be evaluated by first integrating in one direction, which yields the results from the codimension-1 impurities, and then integrating along the second direction.

Of more interest is the question of existence of zero energy eigenvalues in the topological regime. Focusing on the two spatial dimensions, so that there are no parallel directions and we are directly probing the local on-site Greens function, we expect that the terms $G(\epsilon)$ and $G_0(\epsilon)$ will diverge close to the band-edge. In fact, these divergences are captured by expanding around the point where the gap is minimal, $k_G$,

\[ |d(k^x, k^y)|^2 = \Delta^2 + a(k^x - k^x_G)^2 + b(k^y - k^y_G)^2 + \ldots \]
The diverging part of the integral is then captured by the integral

\[
\int -\frac{dk^xdk^y}{(2\pi)^2} \frac{1}{2\Delta \delta \epsilon + a(k^x)^2 + b(k^y)^2}
\]

(4.29)

\[
\sim -\int_0^{0^+} \frac{dq}{2\pi \sqrt{ab}} \frac{q}{2\Delta \delta \epsilon + q^2} \sim \log \delta \epsilon \frac{4\pi}{4\pi \sqrt{ab}}.
\]

(4.30)

Hence, \( \mathcal{G}(\epsilon) \sim -\frac{|\Delta|\log \delta \epsilon}{4\pi \sqrt{ab}} \) and \( \mathcal{G}_0(\epsilon) \sim \frac{d_0(k_\parallel)\log \delta \epsilon}{4\pi \sqrt{ab}} \) in proximity of the valence band. If the gap is not at a \( T \)-symmetric point, this automatically implies that the divergences do not cancel and we are left with eigenvalues that all diverge at both band edges, leading to the fact that the Greens functions eigenvalues have to be zero somewhere in the gap.

On the other hand, if the gap is at a symmetric point we need an extra argument to arrive at the result of the right panel of Fig. 4.4, hence consider \( 0 < m < \frac{1}{2} \). It is straightforwardly seen that \( \mathcal{G}(\epsilon) > 0 \) for \( \epsilon < 0 \) and \( \mathcal{G}(\epsilon = 0) = 0 \). At the same time, we know that both \( \mathcal{G}_0(\epsilon) \) and \( \mathcal{G}(\epsilon) \) have a logarithmic divergence at the valence band. However, as \( d_0(k = 0) > 0 \), the function \( \mathcal{G}_0(\epsilon) \) now goes to negative infinity. At the same time, \( \mathcal{G}(\epsilon) \) goes to positive infinity because in that case the numerator is \( \epsilon < 0 \).

Thus the two lines must cross if \( \mathcal{G}_0(\epsilon = 0) > 0 \), showing that there is consequently a point where \( G_0 \) has zero eigenvalues.

Finally, it remains to prove that, in this construction, \( \mathcal{G}_0(\epsilon = 0) > 0 \) for \( 0 < m < \frac{1}{2} \).

This actually straightforward. Since \( \mathcal{G}_0(\epsilon = 0) = \int \frac{dk_\parallel}{2\pi} g_0(\epsilon = 0, k_\parallel) \) we directly infer that

\[
g_0(\epsilon = 0, k_\parallel) = (m - 4 + 2\cos k_\parallel) \int \frac{dk_\perp}{2\pi} \frac{1}{|d(k_\parallel, k_\perp)|^2} > 0
\]

(4.31)

for all \( k_\parallel \) given \( m < 2 \), and hence \( \mathcal{G}_0(\epsilon = 0) > 0 \) in the desired region \( 0 < m < \frac{1}{2} \).