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Transport Signatures Of Quantum Phase Transitions And The Interplay Of Geometry And Topology In Nodal Materials

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Transport Signatures Of Quantum Phase Transitions And The Interplay Of Geometry And Topology In Nodal Materials

Abstract

The research presented in this thesis is divided into two parts. In the first part, we propose response signatures for quantum phase transitions in superconducting and bilayer graphene systems. In superconducting systems, there is the promise for realizing a Majorana quasiparticle: a fermion that is its own antiparticle and possesses some of the non-Abelian braiding statistics required to form a topological quantum computer. We propose conductance and noise signatures showing the presence of Majorana fermions in topological insulator-superconductor heterostructure Josephson Junctions. We then move on to address the possibility of realizing the physics of quantum point contacts in graphene bilayers. There have been numerous theoretical proposals of quasi-topological domain walls in bilayer graphene. Using bosonization and renormalization group considerations, we propose transport signatures characterizing the pinch-off behavior of the effective point contact formed by the intersection of two domain walls.

In the second part of this thesis, we provide several examples of nodal band features protected by the combination of topology and crystalline geometry. Nodal features in condensed matter systems manifest when the Fermi surface consists only of a limited set of band-touching points with fixed dispersion. The low-energy theories of these touching points resemble those in particle physics, and these nodes, such as the quintessential examples in graphene, are therefore frequently characterized with names such as Dirac and Weyl fermions. The presence of nodal band features at the Fermi energy can have unique implications for bulk transport and surface physics, and so there has been a great effort in recent years to find new theoretical and real-material examples of nodal systems. We begin by showing that when spin-orbit interaction is weak, the same $Z_2$ invariant that predicts a topological insulator can be used when inversion symmetry is present to predict topological Dirac line nodes in crystal systems. On the surface of these line node semimetals, the projected interior of the line nodes can host a two-dimensional nearly-flat band, and could provide a route towards experimental access of phases with significant electron-electron interactions. We then present the first known example of a nodal condensed matter system with a description beyond particle physics: the double Dirac semimetal. In these systems, eightfold-degenerate linearly-dispersing nodal points manifest at the Brillouin zone edge. We list all possible space groups that can host double Dirac points when spin-orbit interaction is non-negligible, and we show that the expanded set of time-reversal-symmetric mass terms for these new fermions allows for new routes towards strain-engineering topological phase transitions and also provides the possibility of topologically-nontrivial line defects. We then move on to two dimensions, for which we use a consideration of compact flat manifolds to deduce all possible manifestations of nodal physics in strong spin-orbit systems. Through this analysis, we explain in more general terms some of the more exotic examples of nodal systems proposed over the past few years, and predict new examples in two and three dimensions. Using conclusions from this analysis and specializing to the wallpaper groups, we then show that a consideration of minimal insulating filling allows one to exhaustively characterize all possible topological and topological crystalline insulators. By realizing that the limited set of wallpaper groups constrains the Wilson-loop eigenvalue flows of a three-dimensional bulk insulating crystal, we present the discovery of a new topological crystalline insulator: the topological Dirac insulator. Unlike the surface states of a conventional topological insulator, the surface states of this new insulator are fourfold degenerate, and therefore can be gapped to realize truly topological surface quantum spin Hall domain walls. Finally, we present the first example of a filling-enforced semimetal in a magnetic system. By exploiting the modified time-reversal symmetry in certain antiferromagnetic systems, we characterize a new class of two-dimensional magnetic
Dirac semimetals. We show that these semimetals manifest a new quantum critical point between quantum Hall phases, and discuss their place in the context of fermion doubling theorems.

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TRANSPORT SIGNATURES OF QUANTUM PHASE TRANSITIONS AND THE INTERPLAY OF GEOMETRY AND TOPOLOGY IN NODAL MATERIALS

Benjamin J. Wieder

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Acknowledgments

That this thesis is complete, and that it has more than 3 chapters in it, is to me a minor miracle. This fall marks my 23rd semester at Penn as a student or an employee. I stumbled mightily at times throughout this process, and in the end, all I can do is thank the people that picked me up and repeatedly gave me the opportunity to bet on myself. I think the only sensible way to do this is in chronological order, and to therefore not assign weights to the immeasurable support that I received.

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The research presented in this thesis is divided into two parts. In the first part, we propose response signatures for quantum phase transitions in superconducting and bilayer graphene systems. In superconducting systems, there is the promise for realizing a Majorana quasiparticle: a fermion that is its own antiparticle and possesses some of the non-Abelian braiding statistics required to form a topological quantum computer. We propose conductance and noise signatures showing the presence of Majorana fermions in topological insulator-superconductor heterostructure Josephson Junctions. We then move on to address the possibility of realizing the physics of quantum point contacts in graphene bilayers. There have been numerous theoretical proposals of quasi-topological domain walls in bilayer graphene. Using bosonization and renormalization group considerations, we propose transport signatures characterizing the pinch-off behavior of the effective point contact formed by the intersection of two domain walls.
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tions and also provides the possibility of topologically-nontrivial line defects. We then move on to two dimensions, for which we use a consideration of compact flat manifolds to deduce all possible manifestations of nodal physics in strong spin-orbit systems. Through this analysis, we explain in more general terms some of the more exotic examples of nodal systems proposed over the past few years, and predict new examples in two and three dimensions. Using conclusions from this analysis and specializing to the wallpaper groups, we then show that a consideration of minimal insulating filling allows one to exhaustively characterize all possible topological and topological crystalline insulators. By realizing that the limited set of wallpaper groups constrains the Wilson-loop eigenvalue flows of a three-dimensional bulk insulating crystal, we present the discovery of a new topological crystalline insulator: the topological Dirac insulator. Unlike the surface states of a conventional topological insulator, the surface states of this new insulator are fourfold degenerate, and therefore can be gapped to realize truly topological surface quantum spin Hall domain walls. Finally, we present the first example of a filling-enforced semimetal in a magnetic system. By exploiting the modified time-reversal symmetry in certain antiferromagnetic systems, we characterize a new class of two-dimensional magnetic Dirac semimetals. We show that these semimetals manifest a new quantum critical point between quantum Hall phases, and discuss their place in the context of fermion doubling theorems.
3.7.1.2 Quantum Critical Point Stability .......................... 127

3.7.2 Resolving the Fixed Line in the U(2) Symmetric Case .... 129

3.7.2.1 Deriving the Euclidean Action for the $T_0 = 1, T_{\pi} = 0$
M-Phase Fixed Point ............................................. 130

3.7.2.2 Cubic-Order Fixed Points about the M Phase for
$g_- \approx 1$ ....................................................... 140

II Topology and Geometry in Nodal Materials 146

4 Dirac Line Nodes in Inversion-Symmetric Crystals with Weak Spin-
Orbit Coupling 147

4.1 Abstract ..................................................... 147

4.2 Introduction .................................................. 148

4.3 Topological Protection of Line Nodes under $I$ and $T$ ........... 150

4.4 Line Nodes in Cu$_3$N .......................................... 152

4.5 Chapter Acknowledgments ..................................... 160

4.6 Supplemental Material ........................................ 160

4.6.1 Proof of Eqn 4.3.1 ........................................ 160

4.6.2 $\mathbb{Z}_2$ topological invariants and Dirac line nodes of Cu$_3$NZn 162

4.6.3 Band structures beyond Cu$_3$NZn and Cu$_3$NPd ............. 165

5 Double Dirac Semimetals in Three Dimensions 169
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.3.1</td>
<td>Compact Flat Manifolds in Two and Three Dimensions</td>
<td>195</td>
</tr>
<tr>
<td>6.3.2</td>
<td>Minimal Insulating Filling by Kramers’ Theorem</td>
<td>201</td>
</tr>
<tr>
<td>6.4</td>
<td>Band Multiplicity and Eigenvalue Structure in the Layer Groups</td>
<td>205</td>
</tr>
<tr>
<td>6.4.1</td>
<td>Time-Reversal-Invariant Momenta</td>
<td>206</td>
</tr>
<tr>
<td>6.4.2</td>
<td>Crystalline Symmetries</td>
<td>207</td>
</tr>
<tr>
<td>6.4.3</td>
<td>Two- and Four-Fold-Degenerate Band Multiplets</td>
<td>211</td>
</tr>
<tr>
<td>6.5</td>
<td>Semimetals in the Layer Groups</td>
<td>217</td>
</tr>
<tr>
<td>6.5.1</td>
<td>WPVZ Bound of 2</td>
<td>220</td>
</tr>
<tr>
<td>6.5.2</td>
<td>WPVZ Bound of 4</td>
<td>223</td>
</tr>
<tr>
<td>6.5.3</td>
<td>WPVZ Bound of 8</td>
<td>231</td>
</tr>
<tr>
<td>6.6</td>
<td>Discussion</td>
<td>239</td>
</tr>
<tr>
<td>6.7</td>
<td>Chapter Acknowledgments</td>
<td>241</td>
</tr>
<tr>
<td>6.8</td>
<td>Appendix</td>
<td>242</td>
</tr>
<tr>
<td>6.8.1</td>
<td>Further Notes on and Examples of Decimations and Flat-Manifold Placement</td>
<td>242</td>
</tr>
<tr>
<td>6.8.2</td>
<td>Tight-Binding Models</td>
<td>245</td>
</tr>
<tr>
<td>6.8.2.1</td>
<td>Layer Group 37</td>
<td>247</td>
</tr>
<tr>
<td>6.8.2.2</td>
<td>Layer Group 23</td>
<td>249</td>
</tr>
<tr>
<td>6.8.2.3</td>
<td>Layer Group 44</td>
<td>251</td>
</tr>
<tr>
<td>6.8.2.4</td>
<td>Layer Group 21</td>
<td>252</td>
</tr>
</tbody>
</table>
6.8.2.5 Layer Group 17 ................................. 254
6.8.2.6 Layer Group 45 ................................. 256
6.8.2.7 Layer Group 33 ................................. 257
6.8.3 List of Filling Conditions for the 80 Layer Groups ....... 259

7 Topological Dirac Insulators 263

7.1 Abstract ........................................ 263
7.2 Introduction ................................... 264
7.3 Wallpaper Groups $p_{gg}$ and $p_{4g}$ .................... 267
7.4 Discussion ...................................... 274
7.5 Chapter Acknowledgments .......................... 276
7.6 Supplemental Material ............................ 276

7.6.1 Fermion Doubling in 2D Crystals ................... 276

7.6.1.1 2D Fermion Doubling for Two-fold-degenerate linear fermions ......................... 277

7.6.1.2 2D Fermion Doubling for Dirac fermions ...... 280

7.6.2 Symmetries and Degeneracies of Wallpaper Groups $p_{gg}$ and $p_{4g}$ .................. 284

7.6.3 Tight-binding notation .......................... 288

7.6.3.1 Symmetries ................................ 289

7.6.3.2 Projector onto occupied states ............... 290

xvi
7.6.4 Wilson loops .......................... 291
  7.6.4.1 Discretized Wilson loop ................. 293
  7.6.4.2 Effect of time-reversal-like symmetries on the Wilson loop ................. 294
  7.6.4.3 Effect of unitary symmetries that leave $k_z$ invariant .... 296
  7.6.4.4 Effect of unitary symmetries that flips the sign of $k_z$ .... 297
  7.6.5 Topological invariant ....................... 298
    7.6.5.1 Single glide .......................... 298
    7.6.5.2 Two glides ........................... 300
    7.6.5.3 $Z_2$ topological invariant in the presence of inversion symmetry ............... 303
    7.6.5.4 Mirror Chern number in Wallpaper Group $p4g$ .... 305
  7.6.6 Tight-Binding Model and the SSH Limit ................. 307
    7.6.6.1 Tight-Binding Model for Space groups 55 and 127 .... 309
    7.6.6.2 Beyond the SSH Limit ...................... 314
    7.6.6.3 Broken $C_4z$ Phases ...................... 315
    7.6.6.4 Strong Topological Insulating Phases ............... 317

8 Filling-Enforced Magnetic Dirac Semimetals in Two Dimensions 323
  8.1 Abstract ........................................ 323
  8.2 Introduction ....................................... 324
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.3 Magnetic Tight-Binding Models</td>
<td>326</td>
</tr>
<tr>
<td>8.4 Materials Realization</td>
<td>336</td>
</tr>
<tr>
<td>8.5 Discussion</td>
<td>338</td>
</tr>
<tr>
<td>8.6 Chapter Acknowledgments</td>
<td>339</td>
</tr>
</tbody>
</table>

9 Future Directions 340
List of Tables

5.1 Space groups that host DDPs. SGs are indicated in International notation as well as in Shönflies notation, which indicates the crystal system and point group. The momenta $\mathbf{K}$ are listed with symmetry labels for the 8DIRs, as well as for some 4DIRs. The final column indicates the $\mathcal{T}$-invariant vector representations of the point group contained in the tensor product $\Gamma^* \otimes \Gamma$ of the 8DIR at $\mathbf{K}$, indicating that in each case a linear dispersion is generic. . . . . . . . . . . . . 172

5.2 Symmetry generators for SGs 130 and 135, along with their representations in the sublattice-spin space. . . . . . . . . . . . . . . . . 175

5.3 Perturbations to the DDP in SG 135, classified by their symmetry under the $D_{4h}$ point group[26]. The resulting insulating and semimetallic (SM) phases are indicated. . . . . . . . . . . . . . . . . . . 178

6.1 Layer groups allowed placement onto the 3-torus, with minimal insulating fillings of $\nu \in 2\mathbb{Z}$. . . . . . . . . . . . . . . . . . . 260

6.2 Layer groups allowed placement onto only the dicosm, with minimal insulating fillings of $\nu \in 4\mathbb{Z}$. . . . . . . . . . . . . . . . . . . 260

6.3 Layer groups allowed placement onto only the 1st amphicosm, with minimal insulating fillings of $\nu \in 4\mathbb{Z}$. . . . . . . . . . . . . . . 261

6.4 Layer groups allowed placement onto either the dicosm of the 1st amphicosm, with minimal insulating fillings of $\nu \in 4\mathbb{Z}$. . . . . . . . . 262

6.5 Layer groups allowed placement onto either the 1st amphidicosm, with minimal insulating fillings of $\nu \in 8\mathbb{Z}$. . . . . . . . . . . . . . . 262
List of Figures

1.1 In principle, an ideal donut can be deformed into an ideal coffee cup (a) (reproduced from http://youngmathwizards.com/lessons/images/TopologyTransformDonutToCoffeeCup.gif). But maybe donuts have sprinkles and look delicious in a box mushed together (b) or maybe a coffee cup doesn’t have a closed handle (c). It’s possible that this imagery does not actually help convey to a general audience that the manifold defined by the Hamiltonian parameterized by the crystal momenta of a topological insulator has an odd genus...

2.1 (a) Three-terminal ring geometry, in which the phase difference across a linear S-TI-S Josephson junction is controlled by the magnetic flux $\Phi$ through the ring. Measurement of the current and low-frequency noise provides a signature sensitive to Majorana fermion modes on the junction.

2.2 Schematic of the 1D Majorana modes that propagate along the junction for $\varphi \sim \pi$, connecting reservoirs on the inside and outside of the ring. A mass term $\Delta_0 \cos(\varphi/2)$ couples the counterpropagating Majorana modes. The transmitted mode at $\varphi = \pi$ defines a single Majorana mode in both contacts. The other Majorana modes in the contacts will be reflected, and characterized by reflection matrices $\tilde{R}_1$ and $\tilde{R}_2$.

2.3 Conductance as a function of $\varphi$ in the single-channel limit. The green curves represent the ideal case for zero temperature and zero voltage in each lead with $\Delta \epsilon = 0.05\Delta_0$. The purple, orange, blue, and red curves respectively represent the cases for $\Delta \epsilon/\Delta_0 = 0.5, 0.2, 0.1,$ and $0.05$ with $T = 0.005\Delta_0$ and $eV_1 = eV_2 = eV = 0.05\Delta_0$.
2.4 Cross noise power $P^{12}$ as a function of $\varphi$ in the single-channel limit. The green curves represent the ideal case for zero temperature and zero voltage in each lead with $\Delta \epsilon = 0.05\Delta_0$. The purple, orange, blue, and red curves respectively represent the cases for $\Delta \epsilon / \Delta_0 = 0.5, 0.2, 0.1, \text{and } 0.05$ with $T = 0.005\Delta_0$ and $eV_1 = eV_2 = eV = 0.05\Delta_0$.

2.5 Cross noise and diagonal noise at $\varphi = \pi$ in the single-channel limit. The green curves represent the ideal case for zero temperature and zero voltage in each lead. The purple, orange, blue, and red curves respectively represent the cases for $T / \Delta_0 = 0.1, 0.05, 0.02, \text{and } 0.005$ with $eV_1 = 0.05\Delta_0$ and $\Delta \epsilon = 0.1\Delta_0$.

3.1 Domain walls in bilayer graphene can be induced by applying a perpendicular electric field and varying either the interlayer stacking (a) or the electric field direction (b). Both kinds of domain walls (the dotted lines) have similar domain wall band structures (c) when the Fermi energy $E_F$ is near the chiral symmetric point. Adopting the notation of Ref. 110, the two domain wall states in each direction are labeled 0 and $\pi$ working from the Brillouin zone edge in. When the Fermi energy is exactly in the middle of the bulk gap, the Fermi velocities are the same for the 0 and $\pi$ bands and electron direction is set by valley index $K/K'$. 

3.2 (a) Two parallel domain walls in bilayer graphene can be created by varying either the interlayer stacking or the perpendicular field direction between regions A and B. (b) Distorting region B such that the walls approach each other results in the equivalent of a Quantum Point Contact (QPC) for the domain wall modes. The numbers 1–4 are lead indexes and the two modes displayed for each domain wall are those at 0 and at $\pi$. All of the modes shown here are at valley $K$; a counterpropagating set of modes exists at $K'$ and is related by time-reversal symmetry. Including electron spin, there are 4 modes in each valley in each domain wall, for a total of 16 modes to consider for this QPC structure.
3.3 Schematic of the valley-preserving single-particle tunneling processes. Many-body processes which conserve spin and valley can be constructed as products of these processes. Among the processes which conserve valley, only spin-conserving processes can become relevant and destabilize the fully pinched-off II $(t)$ and fully-open $(v)$ CC phases, due to the nature of the scaling dimension calculation. For each process about the charge and valley conducting phase $(a)$, there is a dual process about the charge and valley insulating phase $(b)$. The diagram here depicts modes for only a single spin direction; the full QPC hosts an additional set of modes related by a spin flip.

3.4 The regions in interaction space for which tunneling processes become relevant ($\Delta < 1$ in Eqs. (3.3.28) and (3.3.30)) and the fully open (CC) or pinched-off (II) junction phases are destabilized. The central dot at $g_+ = g_- = 1$ is the noninteracting point and the dotted oval is the region of predicted accessible interaction strength in Ref. 110 for a suspended sample. The IC (CI) regions are characterized by four-body tunneling processes which transmit exclusively valley (charge) across the junction. The B regions represent relevant eight-body tunneling processes which are charge insulating $(\pm)$ or conducting $(\mp)$ and differ by band-index and valley-transmission character. Regions of overlap between boundaries, denoted with $\ast$, have multiple relevant operators at different orders and presumably more complicated behavior. In the central region, the fully open (CC) or pinched-off (II) phases remain stable and the conductance is characterized by single-electron tunneling.

3.5 The eight angular variables in the full formulation of the S-matrix, seven of which are linearly independent. $\theta_i$ corresponds to the processes which break small-momentum conservation and scatter electrons between the 0 and $\pi$ bands at lead $i$. $\phi_{ij} = \phi_i - \phi_j$ corresponds to the scattering phase acquired tunneling from lead $j$ to lead $i$ at valley $K$. While there are four independent $\theta_i$ angles, there are only three independent $\phi_{ij}$ as only the relative scattering phase matters, such that $\phi_{43} = \phi_{23} - \phi_{21} + \phi_{41}$. We have only displayed modes at $K$; an additional copy of this picture exists for modes at $K'$, related by time-reversal symmetry. This picture is valid for electrons with either spin, as our model system is SU(2) spin-invariant for all values of charge-sector interaction strengths.
3.6 The two non-zero, non-canceling diagrams for $\mathcal{O}(\epsilon^2_{+/-})$ perturbation theory. Note that $i-l$ are spatial lead indexes and $\alpha-\delta, u-z$ are band indexes which are summed at each vertex over $\epsilon^{\alpha\beta\gamma\delta}$. $\sigma, \sigma'$ are spin indexes for which the $\delta^{\sigma\sigma'}$ within each Green's function has already been taken into account. Even though the system is spin invariant, the spin index on the loop, here $\sigma'$, must still be summed over its two values to calculate the physical RG flow. Each diagram contributes a logarithmic correction to the S-matrix which, when renormalized, leads to a term in Eq. (3.4.12).

3.7 RG flow of the variables $T_{0/\pi}$, which control the pinching off of the junction, calculated to quadratic order in the interactions $\epsilon_{+/-}$ (Eq. (3.4.13)), panels (a)-(c). Large circles correspond to stable fixed points and small circles indicate nontrivial quantum critical points. The flow is controlled by the ratio of the interaction strengths $\epsilon_{-}/\epsilon_{+}$. When $\epsilon_{-}/\epsilon_{+} = 1$, the 0 and $\pi$ bands are completely decoupled and each one behaves individually as a copy of the QSH problem in Ref. 199 (a). For $\epsilon_{-}/\epsilon_{+} > 0$, a set of intermediate fixed points exists which allows the 0 and $\pi$ bands to be pinched off independently (b). When $\epsilon_{-} = 0$, the quadratic theory predicts that a fixed line will exist $T_0 + T_\pi = 1$ (c). Higher-order corrections about this line, calculated in Appendix 3.7.2, infer flow along it back to the central quantum critical point $T_0 = T_\pi = 1/2$ (d).

3.8 A schematic phase diagram, in terms of left-to-right conductance, within the $T_0 - T_\pi$ plane, combining information from Eq. (3.4.13) and Appendix 3.7.2. There are two classes of quantum critical points. The central point controls transitions between the fully open (CC) phase and the fully pinched-off (II) phase. Four additional critical points on the edges control transitions between the CC/II phases and an intermediate mixed (M) phase in which the two bands have differing conductance contributions. The width of the M phase is $\mathcal{O}(\epsilon_{-}/\epsilon_{+})$. 

xxiii
3.9 A reproduction of Figure 3.8 with dashed lines overlaid to indicate possible voltage curves. As the gate voltage $V_G$ winds along a voltage curve, whose exact curvature is dictated by experimental specifics, it passes directly from the II to the CC region along a curve like (a) or indirectly, passing along the way through an intermediate M phase along a curve like (b). At zero temperature, the left-to-right conductance $G_{XX}$ will therefore undergo a direct transition from $0 \rightarrow 8e^2/h$ along (a) or one with an intermediate step up to $4e^2/h$ along (b). This behavior motivates us to search for the finite-temperature scaling of these conductance transitions for $V_G \sim V_{G,A}^*$ (a), or for $V_G \sim V_{G,B}^*$ and $V_G \sim V_{G,C}^*$ (b).

3.10 The two classes of universal scaling functions as functions of external gate voltage: $G_A$ describes the direct II-CC quantum phase transition and $G_B$ describes the II-M transition, plotted in panels (a) and (b) respectively. Here, we have plotted using $\epsilon_+ = 0.212$, $\epsilon_- = 0.071$, such that $\gamma = 1.25$. The curves are plotted for increasing temperature, with the red, orange, green, and blue curves representing $T/c^{3/\alpha} = 0, 10^{-5}, 10^{-2.5}, \text{and} 1 V^{1/\alpha}$ respectively in equations (3.4.24) and (3.4.31). Note that the crossover value of $G_A$ is fixed to be 1/2, whereas the crossover value for $G_B$ is instead at $\gamma/2$, where $\gamma$ varies from 1 to 2 continuously as a function of interaction strength.

3.11 The universal scaling function $G_B$ which characterizes the II-M phase transition, plotted for $T/c^{3/\alpha} = 10^{-3} V^{1/\alpha}$ and $g_+ = 1.212$. The blue, green, orange, and red curves are plotted at $g_- = 1.019, 1.047, 1.071, \text{and} 1.212$ respectively. The critical value of $G_B$ for which the conductance flow changes from the II phase to the M phase occurs at the intersection of each curve with the $\Delta V_G = 0$ line, and varies as a function of the ratio of the interaction strengths $g_-/g_+$. When $g_- = g_+$, $G_B$ takes on the same functional form as $G_A$ in Fig. 3.10, though with a different critical exponent $\alpha_B \neq \alpha_A$. At $T = 0$ K, all of these curves collapse onto the same step function; they are increasingly distinguishable as temperature is increased.

4.1 Crystal structure of Cu$_3$NX. X represents a transition metal atom intercalated at the body-center of the cubic unit cell of Cu$_3$N in an anti-ReO$_3$ structure.
4.2 (color online) Electronic structures and $Z_2$ indices of (a) Cu$_3$NZN and (b) Cu$_3$NPd. Bands are drawn along the high-symmetry lines of the BZ (inset). The Dirac points are indicated by red circles. Parity eigenvalues are illustrated at the eight parity-invariant points in the first octant of the BZ. ........................................ 154

4.3 (color online) Dirac line nodes in the Brillouin Zone (BZ). (a) and (b) Cu$_3$NZN, and (c) and (d) Cu$_3$NPd. The DLNs are illustrated by red curves in the 3D BZ [(a) and (c)] and on the 2D boundary plane of the BZ at $k = X^x$ [(b) and (d)]. ..................... 156

4.4 (color online) Two-dimensional surface electronic structure for Cu$_3$NZN. (a) First octant of three-dimensional Brillouin zone (BZ) of Cu$_3$NZN projected onto the two-dimensional surface BZ of the (100) surface and (b) surface electronic band structure. The Dirac line nodes (DLNs) and the projected interior of DLNs are illustrated with the red and blue schemes, respectively. The slab bands are shown in black lines and surface states in the enclosed region are shown in blue lines. The shaded region represents bulk bands projected onto the BZ of the (100) surface along $k_x$. ............................. 158

4.5 Invariant loop $C_{ab}$ in the Brillouin zone (BZ). The invariant loop $C_{ab} = c_{ab} - \bar{c}_{ab}$ connects two invariant points $\Gamma_a$ and $\Gamma_b$, where $\bar{c}_{ab}$ is a path from $\Gamma_a$ to $\Gamma_b$ along the time-reverse of $c_{ab}$. .................. 161

4.6 Six invariant surfaces $S_{abcd}$ in Cu$_3$NZN. (a) First octant of three-dimensional (3D) BZ. $\xi_i$ of Cu$_3$NZN are presented at parity-invariant momenta $\Gamma_i$, which determine the $Z_2 = (1;111)$ phase. (b) Shaded regions represent three trivial invariant planes (top panel) and three nontrivial invariant planes (bottom panel). ................................. 162

4.7 Dirac line nodes (DLNs) and invariant planes in the BZ of Cu$_3$NZN. Red circles represent the DLNs. The grey-shaded planes illustrate the invariant planes that the DLN at $\Gamma_3$ point ($L_3$) intersects, one of which ($S_{3567}$) is nontrivial and the other two ($S_{0235}$ and $S_{0136}$) are trivial. The intersecting position is depicted by red scheme on the planes. .......................................................... 163

4.8 Invariant loop avoiding intersection with the DLN. The loop $c_{35}$ connecting $\Gamma_3$ and $\Gamma_5$ is bent down in the $-k_z$ direction, while its time-reversed partner $\bar{c}_{35}$ is bent up in the $k_z$ direction. The corresponding interior surface $S_{3567}$ is threaded once by the DLN (illustrated by a red circle). ................................. 164
4.9 Band structures of Cu₃NX, with X={V₀, Ni, Zn}. (a) Cu₃N, (b) Cu₃NNi, and (c) Cu₃NCu. The Dirac nodes are indicated by red circles.

4.10 Band structures of Cu₃NPdx. (a) x = 0.0, (b) x = 0.125, (c) x = 0.25, (d) x = 0.5, (e) x = 0.75, (f) x = 1.0. The Dirac nodes are indicated by red circles.

4.11 Band structures of Cu₃NPd with and without spin–orbit interaction. The bands in the rectangles in (a) are magnified in (b).

5.1 (a) Model lattice for the common tetragonal structure of SGs 130 and 135. The solid lines indicate the four-site unit cell, and solid circles denote the 4 sublattices labeled by (τ², µ²) = (±, ±). (b) Tetragonal Brillouin zone. (c) Energy bands for SG 130, described by the tight-binding model (5.4.1,5.4.5) with tₓᵧ = 1, tᵣ = 0.5 and λ₁ = λ₂ = λ₃ = 0.3. In addition to the DDP at A, there is a symmetry-guaranteed Dirac point on the line Z-R. (b) Bands for SG 135, described by (5.4.1,5.4.6) with tₓᵧ = 1, tᵣ = 0.5, t₁ʹ = t₂ʹ = 0.3, λ₁ʹ = 0.3, λ₂ = 0.1, λ₃ʹ = 0.25. There is a single DDP at A with no other crossings.

5.2 (a) Phase diagram as a function of 3 symmetry-breaking perturbations. A topologically nontrivial loop in the WTI phase is indicated by the dashed circle. (b,c) Uniaxial strain along different directions leads to topologically distinct insulating states. (d) A topological line defect in an insulating state binds a gapless 1D helical mode.

5.3 (a) Band structure of Bi₂AuO₅ in SG 130, obtained from first-principles calculations. The DDP appears at A with extra Dirac points along R-Z. See the supplementary material for the methods.

5.4 Electronic band structure along high–symmetry lines in Bi₂AuO₅ in space group 130.

5.5 Electronic band structure of Sn(PbO₂)₂ in space group 135.

5.6 Electronic band structure of Pb₃O₄ in space group 135.

5.7 Electronic band structure of GaMo₃ in space group 223.
6.1 The 3 compact manifolds which can be achieved by twisting the coordinate-axis-direction boundary conditions for a strictly two-dimensional system that is periodic in both in-plane directions. The local designations of the perpendicular direction are indicated by the arrows, a notation known as the “fundamental polygon.” Of the possible manifolds, the 2-torus (a) and the Klein bottle (b) are flat, but the real projective plane \((RP^2)\) (c) is not. Flatness can be evaluated by testing for the existence of fixed or special points by drawing a circle centered on the boundary and comparing its circumference to that of a circle drawn on the interior. Staring at the bottom left corner, the dashed line indicates the boundary of a circle of radius \(r\). For the 2-torus and the Klein bottle, this boundary explores all four corners, resulting in a circumference of \(2\pi r\), matching the value on the interior. However, for \(RP^2\), this boundary only additionally explores the top right corner before returning, resulting in a reduced circumference of just \(\pi r\), and indicating that the two bottom corners are special points, distinct from the interior and from each other, and therefore that \(RP^2\) is not uniform. The bold numbers indicate the number of times that each pattern would have to be repeated to create a supercell with the same boundary conditions as the initial 2-torus. Pictorial guides to forming such supercells can be found in Appendix 6.8.1.

6.2 The compact, flat manifolds which can be achieved in three-dimensional, layered systems. The notation used is a modification of the fundamental polygon from Figure 6.1 by the additional local assignment of the stacking direction as indicated by the \(\oplus\) and \(\ominus\) signs. Unlike in the strictly two-dimensional wallpaper systems, the modding out of a two-fold screw is also allowed and leads to a new manifold which doesn’t decompose into \(S^1\) multiplied by a wallpaper manifold. Modding out a screw preserves the interior and exterior surfaces leading to the dicosm (b). Modding out a glide reduces the system to being one-sided and leads to the 1st amphicosm (c). In these layered systems, unlike in the 2D wallpaper cases, a particular combination of two perpendicular nonsymorphic operations can be modded out without introducing fixed points, leading to a new flat manifold: the 1st amphidicosm (d). The bold numbers indicate the number of times that each pattern would have to be repeated to create a supercell with the same boundary conditions as the initial 3-torus (a). The procedure for forming such supercells is explained with visuals in Appendix 6.8.1.
6.3 The Su-Schrieffer-Heeger (SSH) Model, tuned to its quantum critical point, on a periodic system. In this limit, the two sublattices are energetically identical, and are therefore related by the nonsymmorphic operation of a mirror of the $y$-direction followed by a half-lattice translation in the $x$-direction. All of the information about this system can be encoded by mandating that both sublattices live at the same potential and by replacing each site with a vector object pointing in the $\pm \hat{y}$ direction (a). When the system has an even number of sites and the boundary condition is not twisted, it lives on a cylinder (b). However, one can produce an electronically equivalent system, if the number of unit cells is large, by removing one site and twisting the axis boundary condition on the $y$ direction, which places the lattice instead on a Möbius strip.

6.4 Possible locations of a glide line $G_y$ relative to an inversion center $I$ ($\otimes$) in a 2D rectangular system with TRIMs $\Gamma XMY$. In both cases, for $T^2 = -1$ all states are two-fold-degenerate because there is a local time-reversal operator $(IT)^2 = -1$. If the inversion center is coincident with the glide line (a), there will be four-fold representations at $X$ and $M$, but all eigenstates of $G_y$ will have eigenvalue pairings $\{+, -\}$ and can never cross. If the inversion center differs from the glide line by a quarter-lattice spacing $a_y/4$ (b), then the operator for $G_y$ will contain an extra $t_y/2$ when defined from the common origin of the inversion center, leading to four-fold points instead at $X$ and $Y$. In this case, then while the bands along $\bar{X}X$ are still paired with $G_y$ eigenvalues $\{+, -\}$, bands along $\bar{Y}M$, if two-fold-degenerate, will be characterized by $G_y$ eigenvalue pairings $\{+, +\}$ or $\{-, -\}$ and can cross and create four-fold Dirac points with local protection [56].

6.5 Four-site model system for semimetals in the layer groups. The four sublattices exist on a 2D rectangular unit cell in the $xy$ plane. Each site has an additional spin degree of freedom. Sites are then each dressed with a 3D vector object, visually represented by the symbols in the inset box, that relates them to their neighbors by a symmorphic symmetry operation and a translation by half a lattice spacing $a_{x/y}/2$. For real systems, this object can represent any time-reversal-symmetric property which transforms as a vector, such as displacement or a local dipole moment. By selecting different A-site vectors and lattice generators, a diverse assortment of semimetallic phenomena can be realized. Hamiltonians are generated by considering all first- and second-nearest neighbor hopping terms permitted by the restrictions imposed on $\mathcal{H}(\vec{k})$ by the generators of a particular layer group. The specific terms allowed for each example layer group are detailed in Appendix 6.8.2.
6.6 The generators (a), lattice (b), and a typical band structure (c) for 
\textit{pmmm}, layer group 37, (space group 47). All elements of the layer 
group are symmorphic, with mirror lines separating the A and B 
sublattices and the A and C sublattices. As the \textit{xy}-plane itself is 
a mirror, this system is flat and has inversion symmetry, with the 
inversion center lying at the center of the four sites and at the inter-
section of all 3 mirror lines and planes. Therefore, by the arguments 
in 6.4.3, bands are two-fold-degenerate with \( M_z \) eigenvalues \{+, −\}. 
Consequently, the bands can only anticross, and at even fillings this 
system is always an insulator (c).

6.7 The generators (a), lattice (b), and a typical band structure (c) for 
\textit{pmm2}, layer group 23, (space group 25). All elements of the layer 
group are symmorphic, with mirror lines separating the A and B 
sublattices and A and C sublattices. The vectors have been bent 
up into the \(+\hat{z}\) direction, breaking \( M_z \) as one would see if there 
were a substrate or a perpendicular electric field added to a system 
in layer group 37 (Fig. 6.6). Consequently, this system is also a 
\textit{wallpaper group}, and could describe the surface of a three-dimensional 
object. Without inversion, nonsymmorphic symmetries, or 
\( n > 2 \) \( C_{n\hat{z}} \) 
rotation points, bands are singly degenerate and can only cross with 
local protection by mirror eigenvalues on the mirror lines. Typical 
values of the tight-binding parameters give metallic states at half-
filling (c), but values can also be chosen to separate the bands into 
groups of two and open up consistent gaps at all even fillings (d).

6.8 The generators (a), lattice (b), and a typical band structure (c) for 
\textit{pbam}, layer group 44, (space group 55). This group is a flat layer 
group generated by constraining into the \textit{xy}-plane a system gener-
ated by two perpendicular screws. Consequently, it has inversion 
symmetry, with the inversion center located in the center of the 
unit cell, off of the glide lines resulting from the product of \( I \) and 
\( S_{2x/y} = t_{x/y} C_{2x/y} \). All bands are at least two-fold-degenerate by 
\((IT)^2 = −1\) and bands along \( XM \) and \( YM \) are four-fold-degenerate 
by the combination of glide mirror and \( M_z \), as detailed in 6.4.3. 
Bands at \( X, Y, \) and \( M \) are four-fold-degenerate due to the relation-
ship between \( I \) and \( S_{2x/y} \), as detailed in 6.4.1 and Ref. 245, and 
disperse linearly. Therefore, at fillings of \( \nu = 2, 6 \), this system is an 
essential Dirac line node semimetal. Two-fold-degenerate bands are 
all paired with \( M_z \) eigenvalues \{+, −\} or in four-fold multiplets with 
\( M_z \) eigenvalues \{+, +, −, −\}, and therefore cannot be tuned to cross 
by band inversion. Consequently, at half filling (\( \nu = 4 \)), this system 
is necessarily an insulator.
6.9 The generators (a), lattice (b), and a typical band structure (c) for $p2_12_12$, layer group 21, (space group 18). This low-symmetry group is generated just by two perpendicular two-fold screws protruding from the sites. Due to having broken inversion symmetry and a combination of nonsymmorphic symmetries incompatible with placement onto the 1st amphidicosm in Fig. 6.2, this system has essential 4-band tangles which resemble hourglasses, such that at fillings of $\nu = 2, 6$, it has 2D essential Weyl points along $\Gamma Y$ and $\Gamma X$ [245]. Bands along most lines are singly degenerate and therefore capable of crossing with symmetry protection by the same mechanism as in Fig. 6.6 (though for the choice of parameters in (c) the system is an insulator at half filling; $\Gamma Y$ is narrowly gapped). Bands along $\overline{XM}$ and $\overline{YM}$ are two-fold-degenerate by the combination of a two-fold nonsymmorphic symmetry and $T$, as detailed in 6.4.3. $M$ hosts four-fold points despite the absence of inversion, owing to $\{S_{2x}, S_{2y}\} = 0$ and $(S_{2x})^2 = (S_{2y})^2 = +1$ at this point, as detailed in 6.4.1. At fillings of $\nu = 2, 6$, this system is therefore an essential semimetal, and can be tuned to have a minimal Fermi surface of four Weyl points and a Dirac point.

6.10 The generators (a), lattice (b), and two possible band structures (c,d) for $p2_1/b11$, layer group 17, (space group 14). The lattice has horizontal glide lines along the sites and inversion centers between the A and C sites and between the B and D sites. Due to the combination of $I$ and $T$, bands everywhere are two-fold-degenerate. The offset between the inversion centers and the glide lines leads to four-fold degeneracies at $X$ and $Y$, as noted in Fig. 6.4 and in 6.4.3. As these four-fold points are linearly dispersing, in accordance with the WPVZ bound this system is an essential Dirac semimetal at fillings of $\nu = 2, 6$, allowing an idealized Fermi surface consisting of two Dirac points. At half filling, however, this system is capable of being both an insulator (c) or a semimetal (d), as bands along $\overline{YM}$ are two-fold-degenerate with pairs of the same glide mirror eigenvalue. This semimetallic phase is locally protected by the statements in Ref. 56, but can be gapped out by a band-inversion transition. Therefore, for guaranteeing the existence of an essential 8-band Dirac semimetallic phase, like that in SrIrO$_3$ in Ref. 34, we find the inversion-center offset highlighted in Ref. 56 to be a necessary, but insufficient condition, and that we must require additional constraints.
6.11 The generators (a), lattice (b), and a typical band structure (c) for \textit{pbma} layer group 45 (space group 57). This high-symmetry layer group has glide mirrors in the $x$ and $z$ directions and $M_y$ about the sites, such that it has an inversion center in the center of its unit cells, off of glide line $G_x = t_y/2M_z$. This offset allows for bands along $XM$ to be two-fold-degenerate with the same $G_x$ eigenvalues, which locally protects Dirac points along that line and its time-reverse, much like the local protection of the Dirac point in Fig. 6.10(d). However, unlike in that previous semimetal, whose nodal features were optionally created by tuning through a band-inversion transition, the Dirac points in layer group 45 are essential, making them more like the essential Dirac line node in SrIrO$_3$ in space group 62 [34]. Because four-fold points are required at $X$ and $M$ by the relationship between $G_x$, $S_y = t_x/2t_y/2C_2y$, and $I$, and because $G_x$ commutes with all other independent symmetry operations of the layer group at $M$, four-fold points at $X$ and $M$ have differing $G_x$ eigenvalue pairings (d), leading to the required crossing along $MX$.

6.12 The generators (a), lattice (b), and a typical band structure (c) for layer group 33 \textit{pb21a} (space group 29). This is the only layer group which can achieve a WPVZ bound of 8 without inversion symmetry. Bands along $\Gamma Y$ are two-fold-degenerate by the anticommutativity of $S_y = t_y/2C_2y$ and $G_x = t_x/2t_y/2M_z$. Bands along $YM$ are two-fold-degenerate by the combination of $G_x$ and $T$. Even though the layer group only consists of two-fold nonsymmorphic symmetries without inversion, the combination of symmetries is such that eight bands have to be tangled together along $\Gamma X$ and $XM$. Listing the eigenvalues of $S_y$ and $G_z = t_x/2M_z$ (d), the evolution of the two-fold nonsymmorphic eigenvalues for each symmetry $\lambda_{\pm} = \pm ie^{ik_x/2}$ causes bands to form characteristic four-band structures as explained in Ref. 245. Starting at $\Gamma$, one can choose parameters such that along $\Gamma X$ there is a gap at half filling with these four-band structures above and below the gap. However, because $[S_y, G_z] = 0$ along $XM$, the four-band structures which form along $XM$ preserve the eigenvalue of $G_z$ ($\pm 1$ indicated as a dashed or solid line respectively) and exchange new partners with local protection, forming a sort of 8-band “cat’s cradle” structure and filling in the gap at $\nu = 4$ with essential Weyl points. Should one tune parameters as to open up a gap along $XM$, the resultant Weyl points at half filling will instead form along $\Gamma X$. 

\[232\]
6.13 A 2-torus (a) and two Klein bottles with a common boundary (b). In order to create a shape with the same external arrows as the 2-torus, two Klein bottles have to be placed together, sharing the common twisted boundary. This procedure is the origin of the bold numbers in Figures 6.1 and 6.2. For a four-site unit cell, this decimation factor, \( n_{\text{dec}} = A_{\text{unit}}/A_{\text{dec}} \) where \( A \) is the area of the original and decimated unit cells respectively, gives the minimal insulating filling constraint \( \nu \in 2n_{\text{dec}}\mathbb{Z} \).

6.14 A demonstration of the decimation procedure for two layer groups with multiple nonsymmorphic symmetries. The minimal insulating filling is proportional to the ratio of the sizes of the maximally decimated unit cell to that of the original, with special consideration given to avoid decimations which introduce fixed points. Layer group 21 (space group 18) (a) is generated by two perpendicular screws: \( S_{x/y} = t_{x/y}/2C_{2x/y} \). One could choose to mod out \( S_x \) first, reducing the area of the unit cell by half and placing the system onto the dicosm. However, further decimation by \( S_y \) would then be disallowed, because \( S_xS_y \sim t_{x/2}t_{y/2}(C_{2z}) \), which is an inherently symmorphic operation \((C_{2z} \text{ about the center of the unit cell})\). Therefore, choosing either screw, the maximal decimation of layer group 21 gives \( n_{\text{dec}} = 2 \) and placement onto the dicosm, with a minimal insulating filling of \( \nu \in 4\mathbb{Z} \). Conversely, layer group 33 (space group 29) (b) is generated by \( S_y \) and \( G_z = t_{x/2}\hat{M}_z \). Modding out \( G_z \) first removes the right half of the unit cell and places the system onto the 1st amphidicosm. However, this is not the maximal decimation, as the product \( S_yG_z \sim t_{x/2}(t_{y/2}\hat{M}_z) \), which is an inherently nonsymmorphic operation. Therefore, layer group 33 admits an additional decimation by \( S_y \) onto the 1st amphidicosm, resulting in \( n_{\text{dec}} = 4 \) and a minimal insulating filling of \( \nu \in 8\mathbb{Z} \).

7.1 Unit cells and Brillouin Zone (BZ) for two-site realizations of wallpaper groups \( pgg \) and \( p4g \), the only two wallpaper groups with multiple nonsymmorphic symmetries. The A and B sites are characterized by \( \mathcal{T} \)-symmetric internal degrees of freedom (blue arrows) that are transformed under crystal symmetry operations. Physically, these could correspond to properties which transform as vectors, such as atom displacements or local electric dipole moments. Glide lines (green) exchange the sublattices. In \( p4g \), there is an extra \( C_4 \) symmetry (⊗) about the surface normal with axes located on the sites. The combination of this \( C_4 \) and the glides produces additional diagonal symmorphic mirror lines (red) in \( p4g \). In the BZ of \( p4g \), \( C_4 \) relates \( \hat{Y} \) to \( \hat{X} \).
7.2 The eight topologically distinct Wilson band connectivities for bulk insulators with crystal surfaces which preserve two orthogonal glide lines. Each band structure is labeled by its two $\mathbb{Z}_4$ indices, $(\chi_x, \chi_y)$, subject to the constraint that $\chi_x - \chi_y = 0 \mod 2$. Under the imposition of $C_{4z}$ symmetry in wallpaper group $p4g$, connectivities are excluded for which $\chi_x \neq \chi_y$. Solid black (dashed blue) lines in the regions $\bar{X} \bar{M}$ and $\bar{\Gamma} \bar{Y}$ indicate bands with $g_x$ eigenvalue $\pm e^{ik_y/2}$, while the solid (dashed) lines in the regions $\bar{Y} \bar{M}$ and $\bar{\Gamma} \bar{X}$ indicate bands with $g_y$ eigenvalue $\pm e^{ik_x/2}$. When inversion symmetry is present, the spectra will be particle-hole symmetric. Bands along $\bar{X} \bar{M} \bar{Y}$ are doubly-degenerate and meet at $\bar{M}$ in a four-fold degenerate point, and bands along $\bar{Y} \bar{\Gamma} \bar{X}$ display either the hourglass (left column) or “double-glide spin Hall” (right column) flows. The (2,0) and (0,2) phases are relatives of the hourglass topologies proposed in Refs. 9, 214. The novel (2,2) topological Dirac insulating phase can host a surface state consisting of a single, four-fold degenerate Dirac fermion.

7.3 The 2D surface Brillouin zone for wallpaper group $p4g$. Bands with glide eigenvalue $\lambda^+ (\lambda^-)$ are drawn as solid (dashed) lines. Bands along lines of type (a) are singly degenerate eigenstates of $g_{x/y}$ and therefore are restricted to either form hourglass or Quantum Spin Hall connectivities along $\bar{\Gamma} \bar{X}$ and $\bar{\Gamma} \bar{Y}$. Along lines of type (b), bands are two-fold degenerate because they are invariant under the combined operation $(g_{y/x} \mathcal{T})^2 = -1$; since such pairs have opposite $g_{x/y}$ eigenvalues, generically lines cannot cross to form four-fold degeneracies at low-symmetry points along this line. However, at (c), the $\bar{M}$ point, bands meet and form a fourfold-degenerate 2D Dirac point. Bands in wallpaper group $p4g$ behave the same way, with the additional restriction from $C_{4z}$ symmetry that bands along $\bar{\Gamma} \bar{X}$ and $\bar{\Gamma} \bar{Y}$ form the same connectivities.
7.4 An example to compute $\chi_y$ according to steps 1-4 in the text. The ± glide sectors are identified by solid black (dashed blue) lines for the bands with $g_y$ eigenvalue $\pm ie^{ik_x/2}$ along $\bar{MY}$ and $\Gamma X$ (analogous labelling is used for the ± glide sectors of $g_x$ along $\bar{Y\Gamma}$.) We now follows steps 1-4 to compute $\chi_y$: 1. Draw the red line labelled $E_1$. 2. One positively-sloped line in the + sector (black solid line) crosses $E_1$ along $\bar{MY}$ and no negatively-sloped lines cross; after multiplying by 2 the total for this step is 2. 3. One positively-sloped line in the + sector (black solid line) crosses $E_1$ along $\bar{\Gamma M}$ and no negatively-sloped lines cross; after multiplying by 2 the total for this step is 2. 4. Along $\bar{Y\Gamma}$, one line with positive slope and one line with negative slope cross $E_1$; the total for this step is zero. The total from steps 2, 3, and 4 is 4. Thus, $\chi_y = 4 \mod 4 = 0$ in this example. We could have also seen that $\chi_y = 0$ by choosing in step 1 the red horizontal line at energy $E_2$. Since no bands cross this line, steps 2-4 again shows that $\chi_y = 0$.

7.5 An example to compute $n_{1\bar{1}0}$ according to steps 1-4 in the text. Along $\bar{\Gamma M}$ the solid black (dashed blue) lines indicate the bands with $m_{1\bar{1}0}$ eigenvalues $\pm i$. Along $\bar{M\bar{X}}(\bar{X}\bar{\Gamma})$ the solid black (dashed blue) lines indicate bands with $g_x(g_y)$ eigenvalue $\pm ie^{ik_y/2}(\pm ie^{ik_x/2})$. To compute steps 1-4, we need only examine the segment $\bar{\Gamma M}$, along which one negatively-sloped line in the + sector and two negatively-sloped lines in the − sector cross the red horizontal reference line. Thus, the result from step 2 is -1, the result from step 3 is -2, and $n_{1\bar{1}0} = 1$. Evaluating $\chi_x$ according to Sec 7.6.5.1 shows that $\chi_x = 1 \mod 2$, examplifying the proof that $\chi_x = n_{1\bar{1}0} \mod 2$.

7.6 The $xz$-plane consisting of $A$ and $C$ sites of the tetragonal lattice for our tight-binding model of space group 127, with lattice spacings $a_{x/z}$ (there is a distinct $xz$-plane consisting of $B$ and $D$ sites that is not visible in this slice). The chains in the $z$-direction can be considered Su-Schrieffer-Heeger (SSH) chains, with hoppings proportional to $u_{1/2}$ dimerizing chains in a strictly $z$-dependent way and hoppings proportional to $v_{1/2}$ coupling sites one lattice spacing $a_x$ (or $a_y$) over so as to introduce $xy$-dependence and allow in $k$-space for terms which manifest at different TRIMs to be tuned independently.
7.7 Energy bands and z-projection Wilson bands for the SSH limit of the tight-binding model for SG 127 in Eq. 7.6.44, with the filling chosen such that the bottom four bands are occupied. Bands (a) and Wilson bands (b) display the trivial connectivity $\chi = 0$ when the polarization invariants at $\bar{X}$ and $\bar{M}$ are the same, and here were obtained using $t_1 = 1, t_2 = 0.5, v_{s2} = -0.2, v_{s2}' = 0.15, u_1 = 0.25, u_2 = 0.45, v_{r1} = v_{s1} = u_3 = u_4 = 0$. When the polarization invariants at $\bar{M}$ and $\bar{X}$ differ, which can be induced by a band inversion about $\bar{M}$ (c), $\chi = 2$ and the Wilson spectrum is nontrivially connected (d). This SSH limit of the topological Dirac insulating phase in SG 127 was obtained using Eq. 7.6.44 with $t_1 = 1, t_2 = 0.5, v_{s2} = -0.2, v_{s2}' = 0.15, u_1 = 0.85, u_2 = 1.3, u_3 = 3, v_{r1} = v_{s1} = u_4 = 0$.

7.8 Bulk bands (a,c) and Wilson bands (b,d) for the tight-binding model (7.6.44) away from the SSH limit. The bands along $\bar{\Gamma} \bar{X}$ open up into hourglasses and the SSH edge states at $\bar{X}$ couple and gap out. For the trivial phase in panel (a), the bottom four bands approach the top four very closely in a few places, but there remains a consistent gap such that the four-band Wilson matrix is well-defined for the whole $z$-surface BZ. Occasionally, an accidental extra symmetry of the tight-binding parameters induces a four-fold degeneracy in the Wilson bands at $\bar{\Gamma}$ in this model (d). These figures were obtained by tuning $v_{r1} \rightarrow 0.55, v_{s1} \rightarrow 0.4$ from the values used in Fig. 7.7 for each phase.

7.9 Bulk bands (a) and Wilson bands (b) for the broken-$C_{4z}$ crystalline phase labelled by $(\chi_x, \chi_y) = (0, 2)$, realized by the tight-binding model of Eq (7.6.44). In this phase, the hourglass along $\bar{\Gamma} \bar{\Gamma}$ is sharply distorted and centered around $\pi$. As occurred for the topological Dirac insulating phase in Fig. 7.8, an accidental extra symmetry of the choice of tight binding parameters can lead to a four-fold Wilson band degeneracy at $\bar{\Gamma}$ (b). The picture was obtained by using the following parameters: $t_1 = 1, v_{r1} = 0.55, v_{s1} = 0.4, t_2 = 0.5, v_{s2} = -0.2, v_{s2}' = 0.35, u_1 = 0.85, u_2 = 1.3, u_3 = 3, u_4 = 4, v_{C4} = 1$.

7.10 Bulk bands (a) and Wilson bands (b) for one of the double-glide QSH phases. This phase can be obtained by adding the term $V_{TI}$ in Eq. 7.6.49 to the Hamiltonian in Eq. 7.6.44 away from the SSH limit. Bands for this figure were generated using $t_1 = 1, v_{r1} = 0.3, v_{s1} = 0.25, t_2 = 1.5, v_{s2} = -0.2, v_{s2}' = 0.15, u_1 = 0.5, u_2 = 2, u_3 = u_4 = 0$, and $v_{TI} = 0.4$.

xxxv
8.1 (a) The lattice with $\mathcal{I}$, $\{M_z|0\frac{1}{2}\}$, and $\mathcal{T} = \{T|\frac{1}{3}\}$ with spins along $\pm \hat{y}$. Red and green indicate sites above and below the plane. (b) The band structure of the system generated by the tight-binding model of Eq. 8.3.2. Bands are two-fold-degenerate by the combination of $\mathcal{I}$ and $\mathcal{T}$. Pictured are the top four bands of an eight-band model, which are split from the bottom bands by a very large antiferromagnetic interaction. The symmetries of this magnetic layer group necessitate that groups of four bands meet in Dirac points at the $M$ point for fillings $\nu \in 4\mathbb{Z} + 2$.

8.2 For the tight-binding model in Eq. 8.3.2, introducing an asymmetry in the interaction between $A/A'$ and $B/B'$ sites may result in edge states on $\mathcal{T}$-preserving surfaces. Pictured above is the (11) edge of a ribbon for different signs of the $M_z$-breaking term $\tau_y$ in the $\mathbf{k} \cdot \mathbf{p}$. The edge shown in (c) and represented by a red line in (a) and (b) above hosts surface states as shown in the inset band structure. The edge in (d), represented by a black line in (a) and (b), is fully gapped. Flipping the sign of $\tau_y$ is equivalent to applying $C_2z$ rotation, which exchanges the two crystalline phases.

8.3 (a) Perturbations corresponding to $\tau_x \sigma_x$ (along with $\tau_x \sigma_y$ and $\tau_x \sigma_z$) result in nodal phases (left) or bulk gapped phases (right), depending on perturbation strength. These cases are associated with dimerizations of the lattice, similar to what’s shown in Fig. 8.2, and may produce edge states in the same fashion (b). $\tau_z$ represents a staggered on-site potential and leads to a pair of Weyl points for small magnitudes (left), two pairs as the magnitude increases (center), and, ultimately, an insulating phase once the Weyl points annihilate (right), but never produces edge states independent of termination. (c) The chiral edge states resulting from breaking $\mathcal{T}$ but preserving the spatial symmetries; left and right moving states sit on opposite edges and connect the valence and bulk manifolds, and are associated with $|C| = 1$. (d) Band structure of the (10) edge of the $\mathcal{T}$-bulk-preserving perturbed system in Fig 8.2. This edge breaks $\mathcal{T}$ and hosts a single, directional trivial edge state, indicating that the $\mathcal{T}$-preserving bulk-insulating phases are Chern-trivial $C = 0$.
8.4 The lattice with $C_{2x}$, $C_{2y}$, and $\bar{T} = \{T^1_{11}\}$. Magnetic moments are along $\pm \hat{y}$. The red and green sites are above and below the plane, respectively; the open-circle site is gray here to indicate that it is in the plane. The symmetries of this magnetic layer group require that bands, while singly degenerate, still group together in multiples of 4 and meet in Dirac points at $M$. Systems in this magnetic layer group are therefore filling-enforced magnetic Dirac semimetals at fillings $\nu \in 4\mathbb{Z} + 2$.

8.5 The band structure of the $\langle 11 \rangle$ edges of a ribbon of the system in Eq. 8.3.3 for (a) a staggered on-site potential and dimerizing interactions with (b) low and high magnitudes. In the latter case, only the termination with unpaired sites (as in Fig. 8.2(c)) is represented. As before, paired edges yield no edge states. Band structures when the bulk is gapped by (c) a $\bar{T}$-breaking term display topological chiral edge states associated with a Chern number $|C| = 1$.

8.6 (a) The structure of an FeSe monolayer. The iron atoms (dark gray) form a planar square lattice, while the selenium atoms sit above and below the plane, so that the iron atoms are tetrahedrally coordinated. Magnetic moments are shown for the striped ordering phase, and are represented by the colored arrows. (b) The band structure of the striped phase of FeSe. Below the Fermi energy, the valence bands form a Dirac point at $M$ that splits weakly along the $M$-$X$ line. The splitting is due to spin-orbit interaction and its weakness is a consequence of the bands comprising primarily iron d-orbitals.
Chapter 1

Introduction

The field of topological condensed matter physics is one of the youngest and most quickly developing areas in physics today. What started in the 1970’s and 80’s as an alternative set of mathematical tools for describing the quantum mechanical version of the Hall effect has, over the past ten years, turned into a veritable gold rush for new topological phases and materials realizations. As the field developed, it grew to incorporate concepts from other areas of physics, including high-energy particle physics and, most recently, crystalline geometry. Despite the field’s growing complexity and specialization, many of its major results can still be understood by making an analogy to the wonder-material graphene. In some sense, graphene is a perfect Dirac semimetal: its Dirac cones are gapless enough to host effective bulk Klein-tunneling and surface states under a valley-preserving termination. But in another sense, it’s actually the world’s worst topological insulator: the presence
of a symmetry-allowed spin-orbit term clarifies insulating filling restrictions and the reveals promise in similar materials of topological insulating physics. In the work presented in this thesis, I have addressed problems across some occasionally disparate areas of quantum condensed matter. However, whether addressing Majorana fermions in superconducting Josephson junctions, the proposed true Dirac cones on a new topological crystalline insulator, or even the domain wall states in actual bilayer graphene, the results derived have simple intuitions drawn from that familiar gapless, or maybe slightly gapped, honeycomb lattice.

In this introduction, we first provide a brief summary of the major results in topological condensed matter physics as they pertain to the discussions in this thesis. We then specialize to considerations of the state of the field before, and after, the major results presented here. In 1.1, we trace the development of topological invariants for quantum Hall systems to the discovery of the first three-dimensional topological insulator. We then in 1.2 discuss the search for condensed matter Majorana fermions, and the relative place of the work presented in Chapter 2. From there, we jump in 1.3 to a discussion of gapped phases in graphene single- and few-layers and the promise for realizing the bilayer graphene domain wall physics presented in Chapter 3.

After providing context for the transport results in this thesis, we then consider progress in the field of bulk nodal materials and topological crystalline insulators. In 1.4, we introduce the weak-spin-orbit Dirac line node from Chapter 4 and briefly
discuss the vast number of similar line node proposals that followed it. In 1.5, we introduce the general notion of minimal insulating filling in time-reversal-symmetric systems and the relationship with so-called “unconventional fermions,” such as the double Dirac points presented in Chapter 5. We then in 1.6 introduce the relatively new field of topological crystalline insulators, touch upon its relationship with the two-dimensional minimal insulating filling restrictions derived in Chapter 6, and explain how the work presented in Chapter 7 closes the search for new time-reversal-symmetric three-dimensional topological insulating phases. Finally in 1.7, we briefly introduce the new magnetic semimetal presented in Chapter 8 in the context of minimal insulating filling and other proposed semimetals.

1.1 A Brief History of Topological Invariants in Condensed Matter Physics

Topology, at least as it applies to condensed matter physics, is the notion that a set of similar problems can share some robustly quantized property as long they are related by smooth deformations. In other words, for some manifold of interest, such as one defined by some mapping of the Hamiltonian of a system parameterized by crystal momenta, we really only care about the genus, or the number of holes, and we can generally ignore other, more complicated math concepts like orientability, at least as long as the manifold has no ill-behaved pointy edges. In practice, this focus
on genus usually leads to introducing this field with pictures of donuts and coffee cups like those in Fig. 1.1, though personally I’m not sure if that does anything but encourage taking a snack break. In this section, we briefly consider the evolution of condensed matter topological invariants from quantum Hall systems to topological insulators and beyond. Much of this story is presented in more detail in a review by Hasan and Kane [83].

In its modern form, the merger of topology and condensed matter theory started upon the recognition that for a Hall bar, a two-dimensional metallic system with an applied in-plane electric field and perpendicular magnetic field, the resistivity is actually a discontinuous function of the strength of the applied voltage. Specifically, in the von Klitzing experiment, the Hall resistivity under increasing voltage was
shown to have well-defined plateaus, whereas the perpendicular, or longitudinal, resistivity was zero except for near the same values of applied voltage at which Hall resistivity jumped [117]. One could consider trying to explain these peaks in the language of single-particle quantum mechanics, beginning with substituting a vector potential into the Hamiltonian for a two-dimensional free particle. The eigenstates of this system then manifest as flat bands, known as Landau levels [119]. In this construction, adding a confining edge potential, like that in the Halperin picture, bends the Landau Levels such that opposite ends appear to host oppositely chiral edge modes [82]. From here, one could propose a semiclassical transport problem where the applied voltage bends the Landau levels and results in the appropriately quantized values of the Hall and longitudinal resistivity. However, a more careful examination of this construction reveals that it only behaves correctly when the Landau levels are fully occupied. To properly characterize the quantum Hall plateaus, one has to in fact introduce a disorder potential that broadens the density of states to include localized modes [218]. In this disordered construction, as the applied voltage is increased, the localized puddles merge until a new set of edge modes eventually appear via a percolation transition [109]. Throughout this process, the Hall resistivity remains quantized up until the percolation transition, and the longitudinal resistivity is zero until the puddles grow so large their edges briefly connect the longitudinal boundaries. Though at each value of applied voltage the details of the disorder-localized puddles differs, the conductivity remains integer quantized.
This edge conductivity robustness led to the recognition by Thouless, Kohmoto, Nightingale, and de Nijs (TKNN) that the voltage change amounts to a continuous deformation of a gapped Hamiltonian with a fixed number of occupied bands; closing and reopening the gap is equivalent to pinching some manifold in such a way that its genus may change [202]. Formulated in the language of Berry’s geometric phase [20], the genus, or in this case the winding number (or 2D Chern number) becomes:

\[
    n_m = \frac{1}{2\pi} \int d^2 k F_m 
\]

where \( F_m \) is the total Berry flux of all the occupied Landau levels. For the quantum Hall problem, TKNN found that \( n_m \in \mathbb{Z} \).

More generally though, the Chern insulator can be considered in terms of its relative lack of symmetries, including, notably, time-reversal symmetry \( \mathcal{T} \). In 1988, Haldane proposed a toy model of the quantum Hall effect on a honeycomb lattice, like the one in graphene [80]. In this model, Haldane encoded the vector potential as \( \mathcal{T} \)-breaking hopping phases that summed to zero across a single unit cell such that the whole 2D system had no magnetic field on the average. This system was found to be capable of hosting \( n_m = 0, \pm 1 \) quantum Hall phases, and stable 2D two-fold-degenerate linearly dispersing fermions at its \( \mathcal{T} \)-symmetric critical points. In 2005, when considering graphene, my advisor Charles Kane and fellow thesis committee member Eugene Mele recognized in a seminal paper that if the Haldane term was
modified to involve the spin degree of system such that it was made $\mathcal{T}$-symmetric, the model would host a tiny gap and robust helical edge modes [106]. After much mathematical heavy lifting, Kane and Mele deduced that these edge modes were protected by a new, time-reversal-symmetric $\mathbb{Z}_2$ variant of the TKNN number, and that therefore their model of graphene represented a new class of “topological insulator.” Shortly afterwards, Bernevig, Hughes, and Zhang recognized that the band inversion in HgTe quantum wells could realize this physics with a much larger gap [19], leading to the observation of this phase via quantized edge conductance in 2007 [118]. From, there, it was a short leap for Fu, Kane, and Mele and Qi, Hughes, and Zhang to propose 3D generalizations of the topological insulator [65, 170]. After a brief time, the surface fermions of these 3D topological insulators were observed in bismuth selenide [93], and by now, a host of other materials [231, 237].

After these developments, Kitaev further noted that, expanding on developments by Altland and Zirnbauer (AZ) in random matrix theory [13], just by counting a Hamiltonian’s number of time-reversal-odd parameters and examining its invariance under a commuting antiunitary operation (time-reversal $\mathcal{T}$) and an anticommuting antiunitary operation (superconducting particle-hole $\Xi$), one could state which topological invariants, if any, could characterize it [115]. Because the quantum Hall state has broken $\mathcal{T}$, no particular sense of particle-hole symmetry, and is two-dimensional, it can automatically be deduced to host an integer-valued topological invariant $n_m \in \mathbb{Z}$. Conversely, the $\mathcal{T}$-symmetric 2D and 3D topological insulators must host $\mathbb{Z}_2$ invariants.
The field then turned towards a broader examination of whether other areas of the Kitaev (or AZ) table, symmetry conditions, or defect structures (Ref. 200, for example) could host readily observable topological phases. In this thesis, we cover two such areas: topological superconducting systems and topological crystalline insulators. As we will see in the following sections, topological superconductors are still quite hard to find and observe. Topological crystalline insulators, on the other hand, were maybe a little too readily characterized and, as shown in Chapter 7, could in fact be exhaustively characterized by a relatively simple consideration of surface symmetries.

1.2 The Search for Condensed Matter Majorana Fermions

The Majorana fermion, a self-dual particle with fermionic algebra, was first proposed 1937 [140]. Much like its namesake theorist, whose disappearance on a boat or appearance on the edge of photos has been the punchline of pretty much every condensed matter talk on the subject [88], the Majorana fermion existed for a long time as more of a curiosity. In particle physics, there has always been the off chance that a neutrino is a Majorana, but otherwise there wasn’t much popular consideration of it until the relatively recent trend of associating the low-energy field theories of condensed-matter systems with particle physics analogs.

In a mean-field superconductor, the many-body operator of the superposition of
adding and removing an electron at zero energy:

\[ \gamma_E = \frac{1}{\sqrt{2}} \left( c_E + c_E^\dagger \right), \ E \to 0 \]  

is self-dual, and of course fermionic. Upon recognizing this, the idea of finding, and finding something useful to do with, a Majorana fermion became a bit less abstract. The most prominent early proposals came from Kitaev, including formulations of Majorana fermions in models of a 1D superconducting chain and on a 2D lattice [113, 116]. As Majorana fermions in 2D are chiral and host anyonic braiding statistics [225, 226], Kitaev’s 2D construction in particular, which also in some form was presented as an exactly solvable model on a honeycomb lattice [114], drew recognition for its proposal for Majorana-based fault-tolerant quantum computing. With Majorana fermions now linked to the search for new superconducting physics and quantum information, attention shifted towards realistic material and device proposals and efforts towards the experimental confirmation of Majorana physics.

The most obvious place to look for robust zero modes, such as Majorana fermions, is in topological systems. The AZ table indicates that there should be topological superconducting systems in two and three dimensions with \( \mathbb{Z} \) or \( \mathbb{Z}_2 \) bulk invariants [13]. Several proposals emerged for effectively realizing these topological superconductors in heterostructure systems, including a proposal by Lutchyn, Sau, and Das Sarma using Rashba wires and superconducting interference devices and a
proposal by Fu and Kane to pattern the surface of a 3D topological insulator with an s-wave superconductor [62, 136].

Efforts to detect elements of topological superconductivity have been ongoing, with some recent success in at least detecting signatures of Majorana fermions [51]. Far and away, the most prominent experimental result came from the Delft group, who in 2012 observed a zero-bias conductance peak in a setup similar to the Lutchyn Rashba proposal [151]. Though this result was eventually confirmed by several groups [43, 46, 47, 58], there was at the time some concern that a similar system without Majorana fermions could nevertheless still display a similar conductance peak [132]. Therefore, there was simultaneously a rush to propose, and construct, devices more reliant on the Fu-Kane topological insulator proximity effect. Following the ambiguous results of a topological-insulator-based setup by the Goldhaber-Gordon group at Stanford [228], we proposed the experimental geometry highlighted in Chapter 2. Shortly afterwards, Yazdani found quite convincing evidence of Majorana fermions in 1D chains of magnetic atoms deposited on superconductors [155]. Partially inspired by Kitaev’s 1D chain, these magnetic atom chains in their superconducting environment were found by scanning-tunneling microscopy to host zero-bias peaks. Of final relevance to this thesis, our Majorana interferometry experiment from Chapter 2 was actually performed in late 2015 [165]. Unfortunately, though that experiment did display conductance signatures of Majorana fermions, the behavior was quite different than what we predicted, and was associated instead with the “snapping” behavior of a Majorana vortex chain living in the non-negligible
channel width of the interferometry device.

1.3 Quasi-Topological Effects in Graphene Few-Layers

Graphene is one of the greatest success stores in hard condensed matter physics. It is a simple system; it consists of a 2D sheet of carbon atoms on a honeycomb lattice and most of its physics can be captured in a spin-orbit-free tight-binding model with just first-neighbor hoppings [35]. Nevertheless, graphene also displays rich electronic physics, some of which can be partially explained exploiting the language of topology. In graphene, the two-fold-degenerate spin-orbit-free bands meet at just two points ($K$ and $K'$) in the Brillouin zone [208]. The bands in these two time-reversed “valleys” disperse linearly; combined with the four-fold degeneracy of these band-touching nodes, this led Semenoff, DiVincenzo, and Mele in 1984 to adopt the language of particle physics and label these points as “massless Dirac fermions” [49, 184]. With a Fermi surface consisting of just these nodes, graphene was found to display ballistic conductance, which could be explained by relating the behavior of electrons in a sublattice-preserving potential to “Klein tunneling” effects in high-energy physics [33, 108]. Furthermore, as long as its edges preserved sublattice labeling (and thus prevented coupling $K$ and $K'$), these bulk Dirac fermions could also be connected with gapless edge modes [28, 66, 156].

As the $\mathcal{T}$-preserving gapped phases of the Dirac equation are topologically dis-
tinct [98], proposals also emerged for gapping graphene and realizing assorted topological effects. Because the spin-orbit coupling in graphene is quite weak, experimental proposals to gap it have relied on patterning substrates or applying external fields. In single-layer graphene, applying a boron-nitride substrate provides an on-site potential that gaps the Dirac points without coupling the valleys (at least to the extent that the two lattices are made perfectly commensurate). In this construction, the different signs of the mass term, corresponding to placing a boron atom on the $A$ or the $B$ sublattice of graphene, correspond to different halves of the Brillouin zone having different Chern numbers [103, 123]. This difference in valley Chern number implies that a domain wall between two oppositely gapped heterostructures should host domain wall states [1, 103]. However, unlike the Chern numbers in the quantum Hall effect discussed in the beginning of this introduction, these Chern numbers are not strictly topological. If the system Hamiltonian is deformed in such a way that the valleys are coupled, then the half-Brillouin-zone Chern number is no longer quantized, and topological edge states are no longer guaranteed. In this sense, I personally consider any discussion of topology in graphene or graphene bilayers “quasi-topological.” While the tools and language of topological condensed matter physics can be used to describe some properties of graphene, one should not get too carried away in proposing a new transport signature that in real systems gets washed out by small, but highly relevant, valley nonconserving disorder.

In light of all of this, the long paper reproduced in Chapter 3 represents an elaborate construction exploiting topological effects at the intersection of similar
domain walls in bilayer graphene. Unlike single-layer graphene, bilayer graphene hosts quadratically dispersing nodes, and can be gapped by a perpendicular electric field [144, 146, 161, 163]. Like in single-layer graphene, these domain walls are only topological if the boundary preserves valley index, and disorder can be highly relevant. Since 2008, these domain walls have been hailed as tunable “highways” for electronic transport in two dimensions [142, 172, 257]. Following a suggestion by Affleck that these domain walls are two-parameter Luttinger liquids [110], we predicted the conductance signatures of pinch-off transitions in the effective quantum point contact at the intersection of two domain walls as a function of interaction strengths [223]. However, to have any hope of observing this transport behavior, there first has to be an experimental confirmation of Luttinger liquid physics in an isolated bilayer graphene domain wall. Progress in this direction has been a mixed bag. Experimental results published in 2015 showed a single-domain wall tunneling conductance approaching the quantized limit of $4e^2/h$, but were inconclusive in displaying the characteristic power law scaling signatures expected for a Luttinger liquid [101]. Recent experiments showed improved domain wall transport, but did not address the Luttinger liquid question [126]. For now, the work presented in Chapter 3 stands as a curious, but possibly too idealized, prediction of another quasi-topological effect in graphene few-layers.
1.4 Weak-Spin-Orbit Line Nodes from Graphite to a Mad Dash for Drumheads

Reproduced in Chapter 4, we presented in 2015 a proof that the same weak and strong invariants that characterize a centrosymmetric topological insulator indicate in weak-spin-orbit crystals the presence of fourfold-degenerate Dirac line nodes [112]. In some sense, each cut piercing one of these line nodes produces 2D Dirac points like graphene; the line node is linearly dispersing in two directions and nondispersing in the third. Previous proposals for similar line nodes had been provided by Volovik and Murakami, but were reliant on either superconducting or artificial sublattice particle-hole symmetries [195, 207]. While our proposed line node is flat under particle-hole symmetry, it survives breaking it, and in fact, survives breaking all symmetries but crystal translation, spinless time-reversal, and spatial inversion. The surface-projected interior of this Dirac line node was also found to host a nearly-flat 2D band. This band, unfortunately dubbed a “drumhead state” in the current literature, has interesting quantum Hall-like effects under an applied magnetic field [152] and, if made sufficiently flat, could provide a vehicle for studying strongly-correlated electron physics.

As we prepared to release our proposal of Cu$_3$N as a Dirac line node semimetal, a competing group was simultaneously preparing papers suggesting these line nodes in graphene superlattices, as well as in the very same Cu$_3$N crystals [220, 247]. In
the end, we both wound up releasing papers roughly simultaneously. During the final week of preparing our paper, the Cava group also informed us that they had found one of these line nodes in a variant of calcium phosphate, a compound Robert Cava now happily refers to as “Dirac Rat Poison” [183]. Given the simplicity of our proposal, that one would likely find Dirac line nodes in weak-spin-orbit systems with band-inversion, a huge number of related line node proposals quickly followed. Most of these line nodes were proposed in space groups with addition mirror symmetries, such that the line nodes could be explained in the language of irreducible representations and mirror eigenvalues [73, 84, 262]. However, a few recent ones were reported in materials simulations of low-symmetry space groups, for which the line nodes could exclusively be described using our topological construction [233, 238].

1.5 Minimal Insulating Filling Semimetals and Unconventional Fermions in Crystals

When presenting at the 2015 March Meeting the Dirac line node proposal reproduced in Chapter 4, we were made aware of a strong-spin-orbit Dirac line node in SrIrO$_3$ [34, 111]. This line node puzzled us for several reasons. First and foremost, we knew from the AZ table that our topological construction could not protect a line node in strong-spin-orbit systems (in which the only valid time-reversal symmetry operator $\mathcal{T}^2 = -1$). Secondly, the papers explaining this strong-spin-orbit
Dirac line node relied on topology and particle-hole symmetry [39], but the line node seemed to be part of eight-band structures that repeated at all fillings, and the system didn’t seem to be particularly particle-hole-symmetric at all. We eventually deduced that this line node was locally protected by the combination of a glide mirror and an inversion center offset from it, a conclusion reported shortly afterwards by Chen Fang in Ref. 56. However, this partial scoop was a bit of a blessing. Looking more closely at the simplified models I had constructed of glides with inversion-center offsets, I realized that not all of them were guaranteed to have eight-band structures; some of them had nodes that could be eliminated by a band-inversion transition.

During the summer after that March meeting, Watanabe, Po, Vishwanath, and Zaletel (WPVZ) released a paper using a consideration of compact flat manifolds to derive the allowed insulating fillings for 220 of the 230 3D space groups [216]. For each of these compact flat manifolds, there was a corresponding space group whose elements all multiplied to operators containing translations. These fixed-point-free space groups, known as the Bieberbach Groups, corresponded to compact flat manifolds in three dimensions, known as the “platycosms” [89]. Bieberbach had in fact characterized this relationship between crystal groups and manifolds as early as a century ago, but the connection to insulating physics had gone unnoticed due to Bieberbach’s subsequent unsavory actions in WWII-era Germany [168]. WPVZ realized that by asking which Bieberbach groups were subgroups of a given space group and imposing Kramers’ theorem, one could quickly predict the fillings at
which most crystal systems were allowed to be insulators. My advisor, Charles Kane, quickly recognized that in the noninteracting limit, this minimal insulating filling would manifest as the number of bands tangled together by space group symmetries. Sure enough, the space group hosting SrIrO$_3$ and its eight-band tangles, space group 62, had minimal insulating fillings of $\nu \in 8\mathbb{Z}$. Exploiting this recognition, we wrote the paper reproduced in Chapter 6, in which we derive the filling restrictions for all two-dimensional systems using a flat manifold-based prescription and predict all of the allowed 2D nodal phenomena for strong spin-orbit interactions. We found both simple 2D systems that reproduced the symmetry protection mechanism of SrIrO$_3$ and new, band-inversion-driven systems protected by the same mechanism, and showed that they were most easily distinguishable by their minimal insulating fillings [221]. Our new band-inversion line node, proposed in a 3D stack of layer group 17 (space group 14), was recently confirmed in density function theoretic calculations by the Balatsky group [70].

At the same time, we also worked to find an explanation for the 10 space groups whose noninteracting minimal insulating fillings were known to be insufficiently constrained by the platycosm formulation. One possibility was that high-fold rotations were enforcing unusually large degeneracies at high-symmetry points. It had been known for some time that a consideration of the dimensionality of the irreducible representation of the Little group at a high-symmetry point would correspond to the degeneracy of the Hamiltonian at that point [139, 244], so we decided to first examine if those space groups hosted unusual irreducible representations. Search-
ing the symmetry textbook Bradley and Cracknell [26], we found that some of the 10 ill-behaved space groups indeed hosted unusual *eightfold-degenerate*, linearly-dispersing nodes, which we dubbed “double Dirac points” [224]. In the work reproduced in Chapter 5, we found that these new double Dirac semimetals allowed new mechanisms for strain engineering quantum phase transitions and could be gapped to bind nontrivial line defects. Following our lead, Bradlyn and the Princeton group used the same methodology to exhaustively characterize all of the possible high-symmetry nodal structures in $\mathcal{T}$-symmetric crystals, discovering in the process so-called “Spin-1 Weyl fermions” [27]. In a soon-to-be-released paper, I collaborated with the Hasan group at Princeton to explore the minimal symmetry restrictions for filling-enforced topological nodal physics. In our upcoming work, we find that in symmorphic chiral crystals, *all* of the time-reversal-invariant crystal momenta host Weyl points, allowing for the potential observation of Brillouin zone-wide Fermi arcs.

1.6 Completing the Menagerie of Topological Crystalline Insulators

Though 3D topological insulators are frequently characterized in terms of bulk time-reversal symmetry, they could also be considered in terms of surface symmetry. Specifically, any facet of a crystal, as long as it is defect-free, is itself some
lower-dimensional crystal. In the case of topological insulators, this surface crystal need only have translation and time-reversal symmetries to host two-fold degeneracies at its surface time-reversal-invariant momenta. As the bands in this 2D subsystem are allowed to be connected to a 3D bulk, they have the added ability to be patterned in an infinite zig-zag connectivity. Therefore, an alternate proposal for 3D topological insulators might go as follows: consider a low-symmetry surface with only translation and $T$ symmetry, rearrange the surface bands so that they have a connectivity that would go on forever without a bulk to absorb it, and ask whether this band connectivity is permitted in a 3D bulk insulator.

Through this alternate prescription, other surface symmetries can also be imposed. In 2008, Teo, Fu, and Kane showed that a symmorphic surface mirror line can protect additional nontrivial surface band connectivities [201]. These bands were shown to be characterized by a bulk mirror Chern number $Z$ and the nontrivial bulk insulating phase was dubbed a “topological crystalline insulator” [60, 201]. By 2012, topological crystalline insulating surface states had been confirmed in SnTe [94, 196] and related materials [50, 234]. As other groups considered the role of multiple mirrors and related effects in phonon systems, the Princeton group in 2015 discovered a nontrivial crystalline insulator protected by a nonsymmorphic glide mirror in density functional theoretic simulations of KHgSb and related compounds [214]. Taking note of the characteristic four-band structures that arise from the combination of glide mirror and time-reversal symmetries in strong-spin-orbit systems, they dubbed this phase a topological “hourglass insulator” [9]. This year,
the existence of the surface hourglass fermions in these materials was preliminarily confirmed through spectroscopy [138].

Shortly after the announcement of hourglass insulators, I realized that by combining the 2D minimal insulating filling considerations from Chapter 6 with the extremely limited set of allowed surface symmetries in \( \mathcal{T} \)-symmetric crystals, one could completely exhaust all of the allowed topological insulating phases, crystalline or otherwise. The trivial surface states in any \( \mathcal{T} \)-symmetric bulk insulator must display the same filling-enforced band tangles as those presented in Chapter 6, and can only come in sets of 2 or 4. Working with Bernevig and Bradlyn, we showed that among the 17 surface wallpaper groups (also known as plane groups) [44], there were generically only four possible kinds of \( \mathcal{T} \)-symmetric topological insulators. Three of them; topological insulators, mirror topological crystalline insulators, and topological hourglass insulators; had already been characterized. But, in the preprint reproduced in Chapter 7, we show that there exists a previously uncharacterized topological insulating phase with \textit{fourfold}-degenerate surface Dirac points. Detailed in Chapter 7, the surface states of this “topological Dirac insulator” are capable of being gapped into truly topological domain wall networks (unlike the ones in bilayer graphene considered in Chapter 3), and also provide important exceptions to a 2D crystalline fermion doubling theorem.
1.7 Magnetic Semimetals

With all of the 3D $\mathcal{T}$-symmetric bulk fermions characterized by the work reproduced in Chapter 5 and Ref. 27, and all of the allowed 3D $\mathcal{T}$-symmetric bulk insulators exhausted by the work reproduced in Chapter 7, a natural question to ask was, “is anything interesting left?” While I can’t answer that question beyond the next year, the work reproduced in Chapter 8 at least provides a glimpse in one possible remaining direction. The platycosm-based formulation of minimal insulating filling presented by WPVZ [216] and adopted for the work reproduced in Chapter 6 only works for time-reversal-symmetric crystals. There are in fact over 1600 magnetic space groups characterizing crystals with broken or modified $\mathcal{T}$ symmetry [128]. In these space groups, there is the likely possibility of finding a rich assortment of unconventional magnetic fermions analogous those in Chapter 5 and Ref. 27, as well as some hope of finding exotic filling-enforced magnetic semimetals analogous to those presented in Chapter 6.

This past year, Steve Young and I took the first steps in this direction: in the paper reproduced in Chapter 8, we showed that in two dimensions, the combination of symmorphic symmetries and an antiferromagnetic time-reversal symmetry protects fourfold-degenerate magnetic Dirac points. These new Dirac points are parts of filling-enforced four-band tangles, and therefore we showed for the first time that insulating filling restrictions greater than $\nu \in 2\mathbb{Z}$ could be achieved without time-reversal symmetry. It is my hope that this new filling-enforced magnetic Dirac
semimetal is only the beginning of a wave of nodal physics discoveries in magnetic systems.
Part I

Transport Signatures of Quantum Phase Transitions
Chapter 2

Signatures of Majorana Fermions in Topological Insulator Josephson Junction Devices

2.1 Abstract

We study theoretically the electrical current and low-frequency noise for a linear Josephson junction structure on a topological insulator, in which the superconductor forms a closed ring and currents are injected from normal regions inside and outside the ring. We find that this geometry offers a signature for the presence of gapless 1D Majorana fermion modes that are predicted in the channel when the phase
difference $\varphi$, controlled by the magnetic flux through the ring, is $\pi$. We show that for low temperature the linear conductance jumps when $\varphi$ passes through $\pi$, accompanied by non-local correlations between the currents from the inside and outside of the ring. We compute the dependence of these features on temperature, voltage and linear dimensions, and discuss the implications for experiments. This chapter originally appeared as an article by Benjamin J. Wieder, Fan Zhang, and C. L. Kane in Physical Review B in 2014 [222].

2.2 Introduction

There is presently a major effort in condensed matter physics to demonstrate the unique properties of Majorana fermion quasiparticle states associated with topological superconductivity [113, 116, 176]. A promising approach is to utilize proximity effect devices that combine ordinary superconductors with topological insulators or other strong spin-orbit materials to achieve topological superconductivity [12, 62, 136, 164, 182]. Recent experiments on semiconductor nanowires coupled to superconductors observed zero-energy tunneling resonances that have been interpreted as Majorana bound states [46, 47, 151, 178]. The original proposal involved a superconductor coupled to the surface of a topological insulator (TI). It was shown that a vortex in the superconductor is associated with a Majorana bound state, and that a linear Josephson junction (JJ) exhibits gapless 1D Majorana fermions when the phase difference is $\varphi = \pi$ [62]. Supercurrents in TI JJ
devices have recently been observed [181, 206, 228]. Unusual behavior, including a smaller than expected critical current normal resistance product, as well as an anomalous Fraunhofer diffraction pattern, has been interpreted as evidence for 1D Majorana fermions along the channel between the superconductors [228]. However, the connection between these observations and Majorana fermions is indirect.

A difficulty with critical current measurements is that the predicted Majorana behavior is only manifest when the phase difference $\varphi$ is close to $\pi$. In order to isolate the properties of the gapless Majorana mode, it is necessary to control the phase. Moreover, the supercurrent carried by the junction includes contributions from gapped states. The gapless mode leads to only a weak singularity in the current phase relation at $\varphi = \pi$. Another possible experiment would be to use a ring geometry and to tunnel into the junction region from another contact. Similar experiments on 1D SNS junctions revealed the expected collapse of the minigap in the normal region for $\varphi = \pi$ [121]. Such experiments on a TI JJ device could demonstrate the closing of the gap, but they would not distinguish an even and odd number of gapless channels. The unique feature of the 1D Majorana mode is that as the phase is tuned through $\pi$, the system must pass through a state where the Majorana mode is transmitted perfectly along the channel - even in the presence of strong disorder. This leads to a quantized thermal conductance that in principle probes the central charge $c = 1/2$ associated with the Majorana mode, but would be difficult to measure.
Figure 2.1: (a) Three-terminal ring geometry, in which the phase difference across a linear S-TI-S Josephson junction is controlled by the magnetic flux $\Phi$ through the ring. Measurement of the current and low-frequency noise provides a signature sensitive to Majorana fermion modes on the junction.

In this chapter we show that measurement of current and low-frequency current noise injected from the normal surface states at the ends of a TI JJ give rise to a unique signature that is sensitive to the perfectly transmitted gapless Majorana mode at $\varphi = \pi$. Our setup, shown in Fig. 2.1, consists of a superconducting ring on the surface of a topological insulator with a linear channel. The phase difference across the junction is controlled by the magnetic flux through the ring, $\varphi = 2\pi\Phi/\phi_0$, with $\phi_0 = \hbar/2e$. In addition, we introduce electrical contacts to the normal TI surfaces inside and outside the ring, as well as to the superconductor. This three-terminal geometry allows the average currents $\langle I^a \rangle$ ($a = 1, 2$) and the correlations $\langle \delta I^a \delta I^b \rangle$ to be measured as functions of the voltages $V^a$ relative to the grounded superconductor. We find that for a long junction at low temperature the linear conductance exhibits sharp steps when $\varphi$ passes through odd multiples of

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1A similar setup may be possible using a 2D Rashba semiconductor proximity effect device[12, 182], though in that case the magnetic field will affect both the flux through the ring and the topological superconductivity.
π. This singular behavior is a direct consequence of the gapless Majorana mode at \( \varphi = \pi \). When the electrical contacts consist of only a single transmitting channel, the magnitude of these steps is \( 2e^2/h \). In the more realistic situation where there are multiple active transmitting channels the singular behavior is still present, though the size of the step is reduced.

In addition, we find signatures for the Majorana mode in the diagonal and cross correlations of the current noise. The cross correlation \( \langle \delta I_1 \delta I_2 \rangle \) exhibits a narrow peak when \( \varphi \sim \pi \) due to the Majorana mode. In the single-channel limit, the height of the peak in the zero temperature limit is universal. For many channels, the peak height is suppressed. The magnitude and sign of the peak, however, is predicted to be related to the size of the steps measured in the average current. Finally, we predict that the diagonal noise correlation \( \langle \delta I_1 \delta I_1 \rangle \) also exhibits a sharp peak at \( \varphi = \pi \). Unlike the singular behavior of the average conductance and the cross correlation, however, the size of the peak is not suppressed when there are many channels, and provides a more robust signature of the Majorana mode.

Our results are related to earlier work concerning resonant transmission through 0D Majorana bound states and proximity effect systems [3, 4, 18, 22, 42, 59, 63, 120, 125, 129, 160, 193, 197, 229]. In particular, Law, Lee and Ng [120] showed that tunneling into a Majorana bound state at \( T = 0 \) leads to a zero-bias resonant conductance \( 2e^2/h \) associated with perfect Andreev reflection of a single channel. In our geometry there are no discrete Majorana zero modes. However, when the
magnetic flux, rounded to the nearest integer multiple of $\phi_0$ is odd, there is effectively a Majorana zero mode inside the ring, but it is strongly coupled to the continuum of states in the surface region coupled to the lead. In this regard, the linear JJ exhibits a behavior similar to the topological transition in a 1D topological superconductor [4]. In our case, the transition between the topological and non-topological phase, which occurs at $\varphi = \pi$ is controlled by the magnetic flux. Noise correlations associated with tunneling into Majorana bound states have also been studied, and the noise correlations for $\varphi = \pi$ resembles the noise correlations that have been studied for coupling to chiral Majorana fermion modes associated with magnet-superconductor interfaces on the surface of a TI [120, 125]. An important difference between the present work and these earlier works, however, is that in our geometry, the superconducting phase $\varphi$, controlled by the magnetic flux through the ring, provides an accessible knob for controlling the coupling between the counterpropagating chiral Majorana modes. This makes it possible to tune through the quantum critical point at $\varphi = \pi$ that separates topological and non-topological phases. An advantage of the present approach is that the singular behavior of the current and noise near $\varphi = \pi$ provides a distinctive signature for the Majorana physics.

The organization of this chapter is as follows. We first present in section 2.3 the specifics of our model for the Josephson junction, focusing on a simple tunneling problem for the Majorana channel and properly treating the interchannel reflection of the remaining modes in the leads. Section 2.4 focuses on experimental signatures
of the gapless Majorana channel: first we discuss the ideal case of single-channel leads and then we expand out to the more realistic multi-channel case, extracting the terms in the multi-channel current and noise which show singular behavior as $\varphi$ winds through $\pi$. Finally, we conclude with a discussion of experimental parameters and feasibility. Additional appendixes 2.7.1 through 2.7.3 provide complete derivations of the multi-channel observables and their single- and many-channel limits.

While the manuscript reproduced in this chapter was in the final stages of preparation we received a preprint by Diez, et al. that presents an analysis of a related Josephson junction geometry for topological superconductors. [48]

### 2.3 Model System

In Ref. 62 it was shown that a Josephson junction on the surface of a topological insulator exhibits a gapless Majorana mode when the phase difference is equal to $\pi$. At that point, there is a single, one-dimensional Majorana mode that is transmitted perfectly along the length of the junction. For $\varphi$ different from $\pi$, a gap opens in that mode. In the following we consider the low energy limit for phase difference close to $\pi$, so that the transmission across the junction is dominated by the single gapless Majorana mode, which can be described by a simple one-dimensional model. As indicated in Fig. 2.2, this mode couples to a single Majorana mode in the contacts
inside and outside the ring. In general, the contacts will involve many additional channels, so it is necessary to introduce a general scattering matrix that relates the incident channels and the transmitted channel.

We begin with a discussion of the one-dimensional transmission problem for the singular channel in 2.3.1 and in 2.3.2 we introduce the general scattering matrix, from which we compute the current and noise as functions of the phase difference $\varphi$, temperature $T$ and the voltages $V^{1,2}$ on the inner and outer contacts relative to the grounded superconductor.

### 2.3.1 One-Dimensional Model

In Ref. 62 a TI JJ was described by modeling the TI surface state by a single massless 2D Dirac fermion coupled to a superconducting pairing potential $\Delta(y) =$
$\Delta_0 \exp(i \text{sgn}(y) \varphi/2)$. For $\varphi \sim \pi$ there are quasiparticle states with $E \sim 0$ bound to the interface $y = 0$ that are described by a two-band Hamiltonian, $H = (\gamma^L, \gamma^R)\mathcal{H}(\gamma^L, \gamma^R)^T$, where the one-body Bogoliubov de Gennes Hamiltonian is 2

$$\mathcal{H} = -i \hbar v_F \sigma^z \partial_x + m(x) \sigma^y. \quad (2.3.1)$$

Here $\gamma^a(x) = \gamma^a(x)^\dagger$ are 1D Majorana fermion operators with $a = L, R$. In this Majorana basis the one-body Hamiltonian $\mathcal{H}$ exhibits particle-hole symmetry $\{H, \Xi\} = 0$ with $\Xi = K$, complex conjugation. The mass term is $m = \Delta_0 \cos \varphi/2$. Importantly, $m$ changes sign when $\varphi$ advances by $2\pi$. In our ring geometry, this means that $\text{sgn}(m) = (-1)^\nu$, where $\nu = \Phi/\phi_0$, rounded to the nearest integer. The mass term violates time-reversal symmetry, expressed by $[\mathcal{H}, \mathcal{T}] = 0$ with $\mathcal{T} = i \sigma^y K$.

For $\varphi = \pi$, $m = 0$, there are uncoupled counterpropagating chiral Majorana fermion modes on the 1D interface.

We should note that the presence of local time-reversal symmetry in the junction at $\varphi = \pi$ obscures the fact that time-reversal symmetry is explicitly broken globally. Furthermore, the physics of this system requires that time-reversal symmetry be broken generally throughout the system. To see this, consider that there is only a single pair of counterpropagating Majorana modes in the junction at $\varphi = \pi$. In a one-dimensional system like this junction, it is not possible to have an odd number of Majorana Kramers pairs without breaking time-reversal symmetry in at least

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2A similar model, describing the transition between a 1D trivial and topological superconductor, has been analyzed in Ref. 4.
some part of the system. Consequently, our system corresponds to symmetry Class D and therefore, even at $\varphi = \pi$, it is appropriate to consider time-reversal symmetry globally broken in our setup [13]. This classification is more than semantic; the restoration of system-wide time-reversal symmetry at $\varphi = \pi$ would generate a second pair of Majorana modes in the junction which would be subject to additional interactions and could alter experimental signatures [48, 256]. Despite the global breaking of time-reversal symmetry, it is worth clarifying that for $\varphi = \pi$, the subsystem of the leads, the junction, and the TI surface linking them does have local time-reversal symmetry. This symmetry prevents the transmitting Majorana mode from being backscattered by non-magnetic disorder. Therefore, one may still analyze moderate disorder in this subsystem by exploiting a time-reversal symmetry, as we later will in 2.4.1. To summarize more precisely, the global breaking of time-reversal symmetry dictates that the junction hosts just a single counterpropagating Majorana Kramers pair at $\varphi = \pi$, whereas the local preservation of time-reversal symmetry protects the transmission of those paired modes into the leads.

To model the ends of the junction, we suppose that $\Delta(x, y)$ varies adiabatically as a function of $x$ and smoothly goes to zero in the lead regions with $|x| > L/2$. In this case each of the 1D Majorana modes in the junction evolves into one of the many propagating channels in the leads. In the spirit of the Landauer-Büttiker approach [31], we focus on this single channel and arrive at a 1D model described by Eq. (5.4.1) for the finite length JJ coupled to the leads. This defines a scattering problem for the chiral Majorana fermion modes incident from the leads.
This scattering problem can be characterized by a $2 \times 2$ $S$ matrix,

$$S_E = \begin{pmatrix} r_1^E & t_2^E \\ t_1^E & r_2^E \end{pmatrix}, \quad (2.3.2)$$

where $t_1^{(2)}$ and $r_1^{(2)}$ describe the amplitudes for transmission and reflection of quasi-particles with energy $E$ incident from the left (right) side. $S_E$ obeys a number of general constraints. Unitarity requires $|r_\alpha^E|^2 + |t_\alpha^E|^2 = 1$ and $|t_1^E|^2 = |t_2^E|^2 = |t_E|^2$. Particle-hole symmetry requires $S_{-E} = S_0^*$. The scattering problem is easily solved for the simple model $m(x) = \theta(L/2 - |x|)\Delta \cos \varphi / 2$. This model has a mirror symmetry ($x \to -x$), under which $S_E \rightarrow \sigma y S_E \sigma y$, so that $t_1^E = t_2^E \equiv t_E$ and $r_1^E = -r_2^E \equiv r_E$. We find

$$t_E = \frac{\hbar v_F \kappa}{\hbar v_F \kappa \cosh \kappa L - iE \sinh \kappa L}, \quad (2.3.3)$$

$$r_E = \frac{m \sinh \kappa L}{\hbar v_F \kappa \cosh \kappa L - iE \sinh \kappa L}, \quad (2.3.4)$$

where $\kappa = \sqrt{E^2 - m^2}/(\hbar v_F)$. At $E = 0$, $S_0$ is real, and is characterized by

$$t_0 = 1 / \cosh(m/\Delta \epsilon), \quad (2.3.5)$$

$$r_0 = \tanh(m/\Delta \epsilon), \quad (2.3.6)$$

where we have defined $\Delta \epsilon = \hbar v_F / L$. For $m \gg \Delta \epsilon$, $r_0 = \pm 1$. Importantly, when $m$ changes sign, $r_0$ changes sign and must pass through zero, at which point the transmission at $E = 0$ is perfect, i.e., $|t_0| = 1$. This property is more general than
our specific model. It is related to the fact that a discrete Majorana zero mode must be present inside the ring for the enclosed flux $\Phi = n\phi_0$ ($\varphi = 2\pi n$) when $n$ is odd, but is absent when $n$ is even. In order for the zero mode to appear or disappear, there must be a point where the gap vanishes and the transmission is perfect for $2\pi n < \varphi < 2\pi(n + 1)$. The perfect resonant transmission is thus a specific signature for a gapless 1D Majorana mode on the junction. However, the transmitted Majorana mode does not carry charge. We will see in the following sections that the transmitted Majorana mode leads to a step in the average current and a peak in the current noise.

### 2.3.2 Current and Noise

We now develop general formulas for the electrical current and noise in our geometry. Similar calculations have been performed previously in Refs. 3, 4, 18, 22, 42, 59, 63, 120, 125, 129, 160, 193, 229. We must combine the transmitted Majorana mode with an additional Majorana mode in each lead as well as properly treat the remaining incident electron channels. For each channel, the Dirac fermion electron operators may be expressed in terms of a pair of Majorana operators,

$$c_E^{a,\alpha} = \gamma_E^{a,\alpha} + i\eta_E^{a,\alpha}, \quad (2.3.7)$$

$$\tilde{c}_E^{a,\alpha} = \tilde{\gamma}_E^{a,\alpha} + i\tilde{\eta}_E^{a,\alpha}, \quad (2.3.8)$$
where \( c_{E}^{α,a} (\tilde{c}_{E}^{α,a}) \) describe modes incoming (outgoing) from lead \( α \) and channel \( a \).

We should note that, in general, a lead \( α \) with \( N^α \) electron channels will have \( 2N^α \) electron and hole channels constrained by particle-hole symmetry. We are free to define our modes such that at \( \varphi = \pi \), \( \gamma^{1α} \) is the extension of the perfectly transmitted mode into the leads. Thus, there is 1 transmitting Majorana channel and \( 2N^α - 1 \) reflected Majorana channels with, in general, no additional constraints.

We can express the relationship between incoming and outgoing Majorana modes in terms of a scattering matrix,

\[
\tilde{\gamma}_E^a = S_{E}^{ab} \gamma_E^b ,
\]

where \( a \) and \( b \) are now indexes for lead, channel, and Majorana type (\( \gamma \) or \( \eta \)) and noting that \( S_{E}^{ab} = S_{-E}^{ba} \) due to particle-hole symmetry. \( S_E \) has the general structure

\[
S_E = \begin{pmatrix}
    r_1^E & t_2^E \\
    t_1^E & r_2^E
\end{pmatrix},
\]

which allowing for only a single transmitting Majorana channel becomes:

\[
\begin{align*}
\tilde{t}_E^α &= \tilde{t}_E^α \ e^{i1} , \\
\tilde{r}_E^α &= \tilde{r}_E^α \ e^{i1} + \tilde{\tilde{r}}_E^α , \\
\tilde{\tilde{r}}_E^α &= \begin{pmatrix}
    0 & 0 \\
    0 & \tilde{\tilde{r}}_E^α
\end{pmatrix} ,
\end{align*}
\]
where $r_\alpha^E$ and $t_\alpha^E$ are single-channel scattering coefficients, $\hat{R}_\alpha$ is a $(2N^\alpha - 1) \times (2N^\alpha - 1)$ dimensional Majorana reflection matrix representing the remaining channels, and $\varepsilon_{ij} = \delta_{ai}\delta_{bj}$. Our plots use for $r_\alpha^E$ and $t_\alpha^E$ the model scattering coefficients in Eq. (2.3.3) and (2.3.4). $S$ and all other matrices for our model are $2(N^1 + N^2) \times 2(N^1 + N^2)$ dimensional.

The operator for the current flowing out of contact $\alpha$ is given by

$$
\hat{I}_\alpha = \frac{e v_F}{L} \sum_E \sum_{a=1}^{N^\alpha} \left( c_{-E}^{a,\alpha} c_{E}^{a,\alpha} - c_{-E}^{a,\alpha \dagger} c_{E}^{a,\alpha} \right)
$$

$$
= \frac{e v_F}{L} \sum_E \left( \gamma_{E}^{\dagger} \Sigma_y^\alpha \gamma_E - \gamma_{E}^{\dagger} \Sigma_y^\alpha \tilde{\gamma}_E \right)
$$

$$
= \frac{e v_F}{L} \sum_E \gamma_a^E A_{ab,\alpha}^E \gamma_b^E, \quad (2.3.14)
$$

where $A_{E}^{\alpha} = \Sigma_y^\alpha - S_{E}^\dagger \Sigma_y^\alpha S_{E}$, $\gamma^\alpha_E$ here is an element of a column vector of Majorana operators in channel $a$, and $\Sigma_y^\alpha = P^\alpha \otimes \sigma_y$, where $P^\alpha$ is a projector onto the modes in lead $\alpha$ and $\sigma_y$ is the Pauli matrix coupling $\gamma^{\alpha,\alpha}$ and $\eta^{\alpha,\alpha}$. Omitted details for this calculation are presented in Appendix 2.7.1. The average current $I_\alpha = \langle \hat{I}_\alpha \rangle$ thus reads

$$
I_\alpha = \frac{e v_F}{L} \sum_E \langle \gamma_{-E}^\alpha \gamma_E^b \rangle A_{ab,\alpha}^E
$$

$$
= \frac{e v_F}{L} \sum_E \text{Tr}[Q_{E}^T A_{E}^\alpha], \quad (2.3.15)
$$
in which we have used the following definition

\[
Q_{E}^{ab} \equiv \langle \gamma_{-E}^{a} \gamma_{E}^{b} \rangle = \frac{1}{4} \sum_{\beta} \left[ f_{E}^{+\beta} P^{\beta} + f_{E}^{-\beta} \Sigma_{y}^{\beta} \right]^{ab}, \tag{2.3.16}
\]

where \( f_{E}^{+\beta} \equiv f^{\beta}(E) \pm [1 - f^{\beta}(-E)] \), the sum and difference of the electron and hole Fermi functions.

Similarly, the low-frequency noise power \( P^{\alpha\beta} = \int_{-\infty}^{\infty} dt \left( \langle \hat{I}_{\alpha}(t) \hat{I}_{\beta}(0) \rangle - I_{\alpha} I_{\beta} \right) \) can be calculated as follows using Wick’s theorem. We find

\[
P^{\alpha\beta} = \frac{e^{2} v_{F}}{L} \sum_{E,E'} \langle \gamma_{-E}^{a} \gamma_{E}^{b} \gamma_{-E'}^{c} \gamma_{E'}^{d} \rangle A_{E}^{ab,\alpha} A_{E'}^{cd,\beta} = \frac{2e^{2} v_{F}}{L} \sum_{E} \text{Tr}[A_{E}^{\alpha} Q_{-E} A_{E}^{\beta} Q_{E}^{T}]. \tag{2.3.17}
\]

The detailed derivation is explained in Appendix 2.7.2.

### 2.4 Experimental Signatures

Here we provide a description of the current and noise observables which characterize the 1D gapless Majorana channel in the JJ. We begin with the average current and conductance at each lead, finding that they are independent of the applied voltage at the other lead and display sharp steps in the low temperature and small voltage limit. We then consider the noise power across the leads and at the same lead. The cross noise signal contains only one term which exhibits a peak at \( \varphi \sim \pi \).
though is suppressed by interchannel scattering. The diagonal noise displays a more complicated signal but exhibits a peak that persists even in the large $N^{1,2}$ limit.

### 2.4.1 Average Current

We will begin with a calculation of the average electric current in the limit that there is only a single channel in the electrical contacts. In principle, this could arise if there was a quantum point contact separating the leads from the surface states. Even away from this limit, however, the simplicity of the result will aid the understanding of the more general results, which we present in the following section.

#### 2.4.1.1 Single-Channel Limit

In the single-channel limit, there is only one additional Majorana mode $\eta^{1,\alpha}$ in each lead, so that $\tilde{R}^\alpha = \pm 1$. Using Eq. (2.3.15) and (2.3.17) and setting $\sum E =
\[ L/(2\pi \hbar v_F) \int_{-\infty}^{+\infty} dE, \]
we obtain

\[ I^\alpha = \frac{e}{2\hbar} \int_{-\infty}^{\infty} dE (1 - r_E^\alpha) f_E^\alpha(E). \]  

(2.4.1)

In Fig. 2.3 we plot the conductance \( G = I/V \) as a function of phase \( \varphi \) predicted by Eq. (2.4.4) for several values of \( \Delta \epsilon \). \( G(\varphi) \) exhibits sharp steps at \( \varphi = 2\pi(n + 1/2) \), provided \( \Delta \epsilon \ll \Delta_0 \). This requirement is equivalent to having the coherence length \( \xi \sim \hbar v_F/\Delta_0 \ll L \), so that quasiparticle tunneling across the superconductor is suppressed for \( \varphi \sim 0 \), leading to perfect normal or Andreev reflection, \( r(\varphi \sim 0) = \pm 1 \). In this limit the width of the step is determined by the maximum of \( \Delta \epsilon \) and \( T \). For \( T \ll \Delta \epsilon \ll \Delta_0 \) the linear conductance is simply,

\[ G(\varphi) = (1 - r_0)e^2/h \]  

(2.4.2)

where from Eq. (2.3.6) \( r_0 = \tanh[(\Delta_0/\Delta \epsilon) \cos \varphi/2] \). \( r_0 \) switches between \(-1\) and +1 over a range \( \delta \varphi \sim \Delta \epsilon/\Delta_0 \ll 1 \), so that over that range \( G \) exhibits a step

\[ \Delta G = 2e^2/h. \]  

(2.4.3)

In the following section we will show that when there are additional channels, the step is still present, but its magnitude is suppressed.

Eq. (2.4.2) can be understood in terms of the four elementary scattering processes for a particle at the Fermi energy incident from one of the leads. The probability
for reflection as an electron (or hole) is $|1 + (-)r_0|^2/4$, while the probabilities for transmission as an electron or as a hole are both $(t_0)^2/4$. For $\Delta \epsilon \ll T \ll \Delta_0$, $G(\varphi) = \tilde{G}(m_\varphi/T)e^2/h$, with $\tilde{G}(X) = 1 - X \int_0^1 dz \sqrt{1 - z^2}/\cosh^2(Xz)$.

### 2.4.1.2 General N-Channel Current

In the general case of many electron channels in each lead we find

$$I^\alpha = \frac{e}{4\hbar} \int_{-\infty}^{+\infty} dE f_E^{-\alpha} \left\{ 2N^\alpha - 2 \text{Re} [r^\alpha_E \tilde{r}^{\alpha}_E] \right\}$$

$$- \text{Tr} [\Sigma_y \tilde{r}^\alpha_E \Sigma_y \tilde{r}^{\alpha}_E].$$

(2.4.4)

This expression contains terms that do not depend on the scattering of the mode that is perfectly transmitted at $\varphi = \pi$. In general, these terms will depend on $\varphi$, but they will not exhibit the singular $\varphi$ dependence associated with the critical mode. Thus, we extract the singular terms, which we denote by $I^\alpha_\gamma$, that depend on $r^\alpha$ and $t^\alpha$.

$$I^\alpha_\gamma = -\frac{e}{2\hbar} \int_{-\infty}^{+\infty} dE f_E^{-\alpha} \left\{ \text{Re} [r^\alpha_E \tilde{r}^{\alpha}_E] \right\}.$$  

(2.4.5)

In the limit $T, V^\alpha \ll \Delta \epsilon$, we have $S_E \approx S_0$. Since $S_E = S_{-E}^*$, $S_0$ is a real, orthogonal matrix. The conductance jump at $\varphi \sim \pi$ due to the step in $r_0$ then becomes

$$\Delta G^\alpha = \frac{2e^2}{\hbar} \tilde{r}^{\alpha}_{22,0}.$$  

(2.4.6)
In general, $\tilde{r}_{22,0}^\alpha$ will depend on the details of the interface between the Josephson junction and the electrical contacts, and can vary in both sign and magnitude. We will not attempt to compute it in detail here. Rather, we will note that the scattering of our system lies somewhere between the limits of a disordered, many-channel quantum point contact and that of a diffusive, quasi-1D conductor. In the limit where the TI surface between the leads and the junction is extremely clean, we can consider, as is done in Ref. 48, that $\tilde{r}_{22,0}^\alpha$ is an element of a $(2N^\alpha - 1) \times (2N^\alpha - 1)$ orthogonal matrix which is, in general, unconstrained by time-reversal or spatial symmetries. Under the assumption that all such matrices are equally likely, the typical value will be $\tilde{r}_{22,0}^\alpha = O(1/\sqrt{N^\alpha})$. Conversely, as is discussed in Ref. 96, we can consider that in the limit that the TI surface linking the lead and the junction has moderate, non-magnetic disorder and has a comparable to that of the elastic mean free path, only a limited number of the electron channels on the TI surface will actively carry current. In this case, only the active channels which penetrate the disorder will be subject to interchannel scattering and the typical value of $\tilde{r}_{22,0}^\alpha$ will be increased to $O(1/\sqrt{N^\alpha_{\text{open}}})$ where $N^\alpha_{\text{open}}$ is on the order of the TI surface conductance in units of $e^2/h$. Since the derivation of the experimental signatures is unchanged between the two limits, we will simplify our notation and redundantly label $N^\alpha_{\text{open}} \equiv N^\alpha$ such that for all intermediate cases

$$\tilde{r}_{22,0}^\alpha = O(1/\sqrt{N^\alpha}).$$

(2.4.7)
Thus, though the magnitude is suppressed, the conductance still exhibits sharp jumps in the limit $T \ll \delta E \ll \Delta_0$. Importantly, the conductances $G^1$ and $G^2$ from the inside and outside leads should exhibit jumps at the same magnetic flux. If observed, these conductance jumps represent a clear signal of a quantum phase transition in the system, corresponding to the insertion or removal of a delocalized Majorana mode in the superconducting ring. The magnitudes and signs of these jumps are each characterized by $\tilde{r}_{22,0}^\alpha$. We will see that the same parameters characterizes the signature in the noise correlations and that the cross noise correlation peaks occur at the same flux as the conductance jumps.

2.4.2 Noise Power

Next we calculate the current-current correlations which contribute to zero-frequency noise power $P^{\alpha\beta}$. We find that the cross correlation $P^{12}$ is characterized be a peak at $\varphi \sim \pi$ due to a single term which corresponds to Majorana transmission across a 1D gapless channel and if detected at half integer multiples of $\phi_0$ gives an unambiguous signature of a quantum phase transition and the insertion of a delocalized Majorana mode into the ring. For a single channel, the peak has a universal height, while, for many channels it is suppressed by the same factors that led to the suppression of the conductance steps. The diagonal noise $P^{\alpha\alpha}$ will be presented in its single-channel and many-channel limits with relevant behavior highlighted. Unlike the cross noise, the diagonal noise contains singular terms which remain as $N^{1,2} \to \infty$. 

43
\[ P^{12} = \frac{e^2}{4\hbar} \int_{-\infty}^{+\infty} dE f_E^{-1} f_E^{-2} r_1^2, \quad \text{(2.4.8)} \]
\[ P^{11} = \frac{e^2}{4\hbar} \int_{-\infty}^{+\infty} dE [1 - r_1^2 f_E^{+1} f_E^{-1}] - (1 - r_1^2 f_E^{-1} f_E^{+1} + |t_E|^2 f_E^{+2} f_E^{-2}). \quad \text{(2.4.9)} \]

\( P^{21} \) and \( P^{22} \) follow from interchanging superscripts 1 \( \leftrightarrow \) 2 in Eq. (2.4.8) and (2.4.9), respectively.

Fig. 2.4 shows the non-local noise correlation \( P^{12}(\varphi) \) evaluated for \( eV_1 = eV_2 = 10T \), for representative values of \( \Delta \varepsilon \). For \( \Delta \varepsilon \ll \Delta_0 \), \( P^{12}(\varphi) \) exhibits a peak near \( \varphi = 2\pi(n+1/2) \). For \( \Delta \varepsilon < T \) the peak height is suppressed by a factor \( \sim \exp(-\pi T/\Delta \varepsilon) \). Observation of the peak in the noise correlations requires \( eV, T \lesssim \Delta \varepsilon \).
In the limit $eV, T \ll \Delta \epsilon$ Eq. (2.4.8) and (2.4.9) reduce to

\[
\tilde{P}_{11} = \frac{e^2}{2h} T \left\{ (t_0)^2 \left[ F\left(\frac{eV^+}{2T}\right) + F\left(\frac{eV^-}{2T}\right) \right] + (1 - r_0)^2 \right\}, \\
\tilde{P}_{12} = \frac{e^2}{2h} T(t_0)^2 \left[ F\left(\frac{eV^+}{2T}\right) - F\left(\frac{eV^-}{2T}\right) \right] 
\]

(2.4.10)  

(2.4.11)

where $F(X) = X \coth(X)$, $V^\pm = V^1 \pm V^2$, and we’ve made the assumption that $t_1^0 = t_2^0 = t_0$ and $r_1^0 = -r_2^0 = r_0$. This assumption is generally valid as most experimental systems in this geometry will be adiabatically connected to our model system in this low-energy limit. This leads to a striking behavior in the zero-temperature limit. For $T \ll V_1, V_2 \ll \Delta \epsilon$, we find that

\[
P^{11} = \frac{e^3}{2h} (t_0)^2 |V_{\text{max}}|, \\
P^{12} = \frac{e^3}{2h} (t_0)^2 V_{\text{min}} \text{sgn}(V_{\text{max}}),
\]

(2.4.12)  

(2.4.13)

where $V_{\text{max}}(V_{\text{min}})$ is the voltage $V^\alpha = 1, 2$ that has the largest (smallest) absolute value.

Obviously the diagonal (off diagonal) noise correlations are sensitive to the maximum (minimum) of the voltages of the leads relative to the superconductor. In Fig. 2.5 we plot the noise correlations at the peak $m = 0$ as a function of $V_2$ for fixed $V_1$ and representative temperatures. The fluctuation in the total current $I^+ = I^1 + I^2$ flowing into the superconductor is given by $P^+ = \langle \delta I^+ \delta I^+ \rangle$ which has
the following simple form:

\[ P^+ = \frac{e^3}{\hbar} t_0^2 |V_1 + V_2|. \]  

(2.4.14)

The current flowing across the junction, \( I^+ = I^1 - I^2 \) has noise \( P^- = \langle \delta I^+ \delta I^- \rangle \) which goes as

\[ P^- = \frac{e^3}{\hbar} t_0^2 |V_1 - V_2|. \]  

(2.4.15)

The features in \( G(\varphi) \) and \( P^{ab}(\varphi) \) near \( \varphi = \pi \), which are predicted to occur over a width \( \delta \varphi \sim \max(\Delta \epsilon, eV, T)/\Delta_0 \) constitute a signature for the Majorana fermion modes associated with the Josephson junction. They are present because over the range \( \delta \varphi \), a Majorana zero mode is transferred from one end of the junction to the
2.4.2.2 N-Channel Generalization of the Noise Power

When there are multiple channels the cross correlation is

\[
P^{12} = P^{12}_\gamma = -\frac{e^2}{4h} \int_{-\infty}^{+\infty} dE f^{-1}_E f^{-2}_E t_{12}^{1*} t_{22,E}^{2*} \tilde{r}_{22,E}^{22,*}
\]

(2.4.16)

In the limit, \(eV, T \ll \Delta\epsilon\), the cross noise still maintains the form of Eqn. (2.4.11) but is suppressed:

\[
\tilde{P}^{12} = \frac{e^2}{2h} T(t_0)^2 \left[ F \left( \frac{eV_+}{2T} \right) - F \left( \frac{eV_-}{2T} \right) \right] \tilde{r}_{22,0}^{12*} \tilde{r}_{22,0}^{22,*}.
\]

(2.4.17)

For \(T \ll V_1, V_2 \ll \Delta\epsilon\), the Fermi functions become step functions and the cross noise becomes

\[
P^{12}(\varphi) = -\frac{e^3 V_{\text{min}}}{2h} \text{sgn}(V_{\text{max}}) t_0^2(\varphi) \tilde{r}_{22,0}^{12} \tilde{r}_{22,0}^{22,*}.
\]

(2.4.18)

which still maintains the same \(V_{\text{min}}, V_{\text{max}}\) dependence as 2.4.13. The height of this peak as a function of \(\varphi\) is related to the conductance jumps in Eq. (2.4.6) by the scattering parameters \(\tilde{r}_{22,0}^{12}\), which can be independently measured using the average current at each lead. Thus, for many channels we expect the cross noise to be suppressed by a factor of order \((1/\sqrt{N_1 N_2})\).
The diagonal noise signal $P^{11}$ has a more complicated dependence on $\varphi$ as well as on the elements of $\tilde{r}^1_E$ and is fully derived in Appendix 2.7.3. However, we find that in the large $N^{1,2}$ limit, in which the $O(1/\sqrt{N^\alpha})$ terms are completely suppressed, there remains a peak in the noise that gives a robust signature for the transmitted Majorana mode. In particular, we find

$$P^{11}_{\text{many}} = \frac{e^2}{4\hbar} \int_{-\infty}^{+\infty} dE \left( f^{+1}_{-E} f^{+1}_{E} \right) \left( 2N^1 - |t_E|^2 \right) + f^{+1}_{-E} f^{+1}_{E} |t_E|^2. \quad (2.4.19)$$

In the $T, V \ll \Delta \epsilon$ limit the singular piece of this becomes

$$P^{11}_{\text{many}, \gamma} = \frac{e^2}{2\hbar} (t_0)^2 T \left\{ F \left( \frac{eV^+}{2T} \right) + F \left( \frac{eV^-}{2T} \right) - F \left( \frac{eV^1}{T} \right) - 1 \right\}. \quad (2.4.20)$$

The voltage dependence of $P^{11}_{\text{many}, \gamma}$ is further clarified in the $T \ll V_1, V_2 \ll \Delta \epsilon$ limit:

$$P^{11}_{\text{many}, \gamma} = \frac{e^3}{2\hbar} (t_0)^2 \left\{ |V_{\text{max}}| - |V^1| \right\} \quad (2.4.21)$$

which vanishes if $|V^1| \geq |V^2|$. This behavior is quite distinctive and gives a clear indicator of a single gapless Majorana channel. There will be a peak in the current in lead 1 due to an applied voltage in lead 2, but no peak if a voltage is only applied to lead 1. In all of these cases, the diagonal noise still contains singular pieces in the large $N^{1,2}$ limit and therefore provides, of all the quantities discussed in this paper, perhaps the most robust signature of gapless Majorana modes.
2.5 Conclusion

In this chapter we have computed the electrical current and noise for a Josephson junction structure on the surface of a topological insulator that allows a clear signature of the gapless Majorana mode, predicted at phase difference $\varphi = \pi$. We predict that the average current exhibits sharp steps as a function of phase difference for a long junction at low temperature and voltage. The diagonal and off diagonal noise correlations exhibit peaks at $\varphi = \pi$. The amplitudes of the singular steps and peaks are predicted to be universal in the case where the electrical contacts couple via a single channel. For $N$ open electron channels, the singularities remain finite, but the current steps are reduced by $1/\sqrt{N}$, while the cross noise correlation is suppressed by $1/N$. The diagonal noise includes a peak that is not suppressed for large $N$.

We now briefly discuss some relevant issues for experimentally implementing our proposal. The number of channels of the leads is an important parameter for determining the lower bound on the size of the singular contributions. For a ring geometry, as in Fig. 2.1, this can be roughly estimated as $N^\alpha \sim k_F R^\alpha$, where $R^\alpha$ is the radius of the inner or outer edge of the ring. To minimize this, it is clearly desirable to control the Fermi energy of the topological insulator surface states, such that the Fermi energy is close to the Dirac point. In this case, $N^\alpha \sim E_F R^\alpha/\hbar v_F$, where $v_F$ is the velocity of the surface states. For Bi$_2$Se$_3$, $\hbar v_F \sim 0.3$ eV nm, so for
Additionally, if there is disorder at the interface between the leads and the junction, the number of active electron channels will be decreased and \( N \) will then go instead as the conductance of the TI surface in units of \( e^2/h \). Typical values for TI surface conductance in these devices range from \( N \sim 20 \) to \( N \sim 200 \) depending on sample purity and efforts to tune the Fermi energy \([190]\). Also, in the presence of disorder, the noncritical part of the conductance will be dependent on effects, such as enhanced reflectionless tunneling or weak localization, which depend on the magnitude of the applied field \([141]\). It is desirable to minimize these aperiodic contributions across the addition of a single \( \pi \)-flux by decreasing the amount of field required to insert one flux quantum. To that end, one should make the cross-sectional area of the ring as big as possible. Equivalently, one should maximize \( H_c A_{\text{ring}}/\phi_0 \) where \( H_c \) is the critical field of the superconductor.

A final key parameter in our theory is the level spacing \( \Delta \epsilon = \hbar v_F/L \). To observe sharp features in the current and noise at \( \varphi = \pi \) we require \( \Delta \epsilon \ll \Delta_0 \), so that \( L \) is larger than the coherence length \( \xi = \hbar v_F/\Delta \). This ensures that for \( \varphi \neq \pi \) the transmission of quasiparticles across the superconductor is exponentially suppressed. Since the noise peak is suppressed for \( \Delta \epsilon < T \), observation of non-local noise correlations requires that \( L \) not be too large. There is ample room to satisfy these constraints experimentally. For example, in Ref. 228 devices with Ti/Al

\[^{3}\text{This rough estimate of } N \sim 10 \text{ also implies a fairly optimistic surface carrier density of } 10^{11} \text{ cm}^{-2}. \text{ The best experiments to date have achieved densities as low as } 10^{12} \text{ cm}^{-2}, \text{ so it is not unrealistic to consider that intermediate values of carrier density will be achieved in improved future TI samples [260].} \]
electrodes ($\Delta_0 \sim 150\mu eV$) were studied. While $v_F$ is not known exactly for these devices, an upper bound is the velocity characterizing the Dirac surface states of Bi$_2$Se$_3$, $\hbar v_F \sim 0.3eV$ nm. This leads to $\xi \lesssim 1.8\mu m$. For longer junctions, in which $L > L_T = \hbar v_F/T$ or the inelastic length $L_{in}$, the noise correlations will be suppressed, but the step in the conductance as well as the diagonal noise peak remain robust, provided the flux through the ring (and hence the phase $\varphi$) can be controlled with the applied magnetic field. For this, it is desirable to minimize the self-inductance $\mathcal{L}$ of the ring, so that the Josephson energy, $E_J \cos 2\pi \Phi/\phi_0$, which tends to quantize the flux, is dominated by $\Phi^2/2\mathcal{L}$. In Ref. 228, devices with $L \sim 1\mu m$ had critical current $I_c \sim 1\mu A$. Using $E_J = \hbar I_c/e$ and $\mathcal{L} \sim 4\pi R \log R/L$ (for a ring of radius $R$ and thickness $L$), we find that this condition is satisfied for $R \lesssim 100\mu m$.

2.6 Chapter Acknowledgments

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2.7 Appendix

2.7.1 Average Current Calculation

For the purpose of clarity, we will work out in detail our derivation of the $N$-channel current and noise, beginning with our choice of a Majorana basis and working in this appendix up to the average current and its single-channel and many-channel limits. Appendixes 2.7.2 and 2.7.3 will expand upon this work up to the general expression for zero-frequency noise power and its forms in the interchannel and same-channel cases.

We begin with the choice of constructing Majorana operators

\begin{align}
\gamma^a_E &= \frac{1}{2} (c^a_E + c^a_{-E}), \\
\eta^a_E &= \frac{i}{2} (c^a_E - c^a_{-E}),
\end{align}

where $a$ represents a given channel and these linear combinations have been chosen such that these new operators are $+1$ eigenstates of the particle-hole operator $\Xi = \tau_x K$ in the electron-hole basis of

\begin{equation}
\psi_E = \begin{pmatrix} c_E \\ c^\dagger_{-E} \end{pmatrix}.
\end{equation}

These operators obey the additional property that $\gamma^\dagger_{-E} = \gamma_E$, such at $E = 0$. 

52
they obey the Majorana relation $\gamma_0^\dagger = \gamma_0$. We note that since our new operators are just linear combinations of electron creation and annihilation operators, they still have canonical anticommutation relations \{\gamma_E^a, \gamma_{E'}^b\} = \delta^{ab}\delta_{E,E'} and still obey Wick’s theorem when calculating higher order correlation functions. The two kinds of Majorana have valid contractions with themselves and between species, leading to four correlators that will be of use:

\[
\langle \gamma_{-E}^a \gamma_{E'}^b \rangle = \langle \eta_{-E}^a \eta_{E'}^b \rangle = \frac{1}{4} f_{E}^\pm \delta^{ab} \delta_{E,E'}, \tag{2.7.4}
\]

\[
\langle \gamma_{-E}^a \eta_{E'}^b \rangle = -\langle \eta_{-E}^a \gamma_{E'}^b \rangle = \frac{i}{4} f_{E}^- \delta^{ab} \delta_{E,E'}, \tag{2.7.5}
\]

where $f_{E}^\pm \equiv f(E) \pm [1 - f(-E)]$ and comes from substituting the definitions of our Majorana operators into the above correlators and noting that $\langle c_{E}^{\alpha \dagger} c_{E'}^b \rangle = f_{E} \delta^{ab} \delta_{E,E'}$ and $\langle c_{-E}^{\alpha \dagger} c_{-E'}^b \rangle = (1 - f_{-E})\delta^{ab} \delta_{E,E'}$, the Fermi distributions for electrons and holes respectively. From here, we can introduce the current operator

\[
\hat{I}^\alpha = \frac{e v_F}{L} \sum_{E} \psi_{-E}^{\alpha \dagger} \Sigma_{E}^{\alpha,ab} \psi_{E}^b - \bar{\psi}_{-E}^{\alpha \dagger} \Sigma_{E}^{\alpha,ab} \bar{\psi}_{E}^b. \tag{2.7.6}
\]

$\Sigma_{E}^{\alpha}$ is the matrix for charge-weighted momentum through lead $\alpha$ in the electron-hole basis and we have expanded $\psi_E$ to be $2(N^1 + N^2)$ dimensional for our two-lead geometry where $N^\alpha$ is the number of channels in lead $\alpha$. The $-E$ for $\psi^{\dagger}$ comes from the delta function in energy that we get by time-averaging and summing over individual operator energies. $\Sigma_{E}^{\alpha} = P^\alpha \hat{\Sigma}$ where $P^\alpha$ is the projection matrix into the subspace of lead $\alpha$ and $\hat{\Sigma} = 1(N^1 + N^2) \otimes \sigma_z$. Rotating this into our Majorana
\[
\hat{I}^\alpha = \frac{e v_F}{L} \sum_E \gamma^\alpha_{-E} \Sigma_y^\alpha \eta^b_{\alpha,ab} \gamma^b_{-E} - \tilde{\gamma}^\alpha_{-E} \Sigma_y^\alpha \eta^b_{\alpha,ab} \gamma^b_{-E}, \quad (2.7.7)
\]

where we should note that \( \gamma^\alpha_E \) is a Majorana of type \( \gamma (\eta) \) for odd (even) \( a \). There will always be an even number of modes since we have artificially doubled the electron channels in each lead as to handle both normal and Andreev reflections off the superconductor. The alternating pattern of entries in \( \gamma_E \) allows us to summarize Eq. (2.7.5) as follows

\[
Q_{\beta,ab}^E \equiv \langle \gamma^\alpha_{-E} \gamma^b_{E} \rangle = \sum_{\beta=1,2} Q_{\beta,ab}^E, \quad (2.7.8)
\]

\[
Q_{\beta,ab}^E = \frac{1}{4} \left[ f^+_{E,\beta} \Sigma^\beta + f^-_{E,\beta} \Sigma_y^\beta \right]^{ab}. \quad (2.7.9)
\]

The outgoing operators \( \tilde{\gamma}^\alpha_E = S_E^a \gamma^b_E \) where \( S_E \) is a \( 2(N^1 + N^2) \times 2(N^1 + N^2) \) dimensional scattering matrix that obeys the property \( S_E = S^*_{-E} \), which can be derived by Hermitian conjugating \( \tilde{\gamma}_E \) and using \( \gamma^\dagger_E = \gamma_{-E} \), and is a consequence of particle-hole symmetry. This allows us to write the current operator in a much more compact form

\[
\hat{I}^\alpha = \frac{e v_F}{L} \sum_E \gamma^\alpha_{-E} A^\alpha_{E} \gamma^b_{E}, \quad (2.7.10)
\]

\[
A^\alpha_E = \Sigma^\alpha_y - S^\dagger_{E} \Sigma^\alpha_y S_E. \quad (2.7.11)
\]

With all of these definitions in place, we can finally begin to take the expectation
value of $\hat{I}^1$:

$$I^1 = \langle \hat{I}^1 \rangle = \frac{e v F}{L} \sum_E \langle \gamma_0^{- E^b} \rangle A^1_{E}$$

$$= \frac{e v F}{L} \sum_E Q_{E}^{ab} A_{E}^{1,ab}$$

$$= \frac{e v F}{L} \sum_E \text{Tr}[Q_{E}^{T} A_{E}^{1}], \quad (2.7.12)$$

which gives us a general average current of

$$I^1 = \frac{e v F}{4L} \sum_E \left\{ f_{E}^{-1} \text{Tr}[P_{E}^{1} - \Sigma_{E}^{1} S_{E}^{1} \Sigma_{E}^{1} S_{E}] ight.$$  

$$+ f_{E}^{+1} \text{Tr}[P_{E}^{1} S_{E}^{1} \Sigma_{E}^{1} S_{E}]$$

$$+ f_{E}^{-2} \text{Tr}[\Sigma_{E}^{2} S_{E}^{1} \Sigma_{E}^{1} S_{E}]$$

$$+ f_{E}^{+2} \text{Tr}[P_{E}^{2} S_{E}^{1} \Sigma_{E}^{1} S_{E}] \right\}. \quad (2.7.13)$$

We can introduce into this a general S-matrix of the form

$$S_{E} = \begin{pmatrix} r_{E}^{1} & \xi_{E}^{2} \\ \xi_{E}^{1} & r_{E}^{2} \end{pmatrix} , \quad (2.7.14)$$

in which unitarity restricts $r_{E}^{\alpha} r_{E}^{\alpha} + \xi_{E}^{\alpha} \xi_{E}^{\alpha} = 1$. The average current now becomes

$$I^1 = \frac{e v F}{4L} \sum_E f_{E}^{-1} \left\{ 2N_{1}^{1} - \text{Tr}[\Sigma_{y} \xi_{E}^{1} \Sigma_{y} r_{E}^{1}] \right\}$$

$$+ f_{E}^{+1} \text{Tr}[\xi_{E}^{1} \Sigma_{y} r_{E}^{1}] + f_{E}^{-2} \text{Tr}[\Sigma_{y} r_{E}^{2} \Sigma_{y} \xi_{E}^{2}]$$

$$+ f_{E}^{+2} \text{Tr}[\xi_{E}^{2} \Sigma_{y} \xi_{E}^{2}] , \quad (2.7.15)$$

55
where we have used $\Sigma_y$ to represent any square matrix of the form $1 \otimes \sigma_y$ and $\Sigma_y^\alpha$ to represent any projection of a matrix of that form. This means that our $\Sigma_y$ matrices will possibly be different sizes; nevertheless they are carefully ordered in such a manner that all matrix products are still valid.

In our Majorana basis, only a single channel may be transmitting, which restricts the form of our $S$ matrix

\begin{align*}
\xi_E^\alpha &= t_E^\alpha e^{11}, \\
\varrho_E^\alpha &= r_E^\alpha e^{11} + \tilde{\varrho}_E^\alpha. \tag{2.7.16, 2.7.17}
\end{align*}

where $r_E^\alpha$ and $t_E^\alpha$ are scattering coefficients for the single transmitting channel and the elements of the matrix $e_{ij}^{ab} = \delta_{ai}\delta_{bj}$. The scattering matrices for the remaining channels $\tilde{r}_E^1 \neq \tilde{r}_E^2$ are in general unequal as the leads differ in channel number and structure and are otherwise unrelated by additional symmetries. These matrices have the structure

\begin{equation}
\tilde{\varrho}_E^\alpha = \begin{pmatrix}
0 & 0^T \\
\vec{0} & \tilde{R}_E^\alpha
\end{pmatrix}, \tag{2.7.18}
\end{equation}

where $\vec{0}$ is the zero column vector and $\tilde{R}_E^\alpha$ is an undetermined $(2N^{\alpha} - 1) \times (2N^{\alpha} - 1)$ dimensional reflection matrix. $\tilde{R}_E^\alpha$, as discussed in 2.3.1, is unconstrained by time-reversal symmetry for $\varphi \neq \pi$. Additionally, due to the presence of some possible disorder and the underlying unusual ring geometry, the reflection matrices are also in the most general case unconstrained by spatial symmetries. The presence of
disorder may also reduce the number of channels which participate in interchannel
scattering, effectively sending $N^\alpha \to N_{\text{open}}^\alpha$, where $N_{\text{open}}^\alpha$ is the number of transmit-
ting electron channels through the disorder on the TI surface between the leads
and the junction [96]. Noting that $t_{E}^{\alpha \dagger} \Sigma y_{E} t_{E}^{\alpha} = 0$ and $\Sigma y_{E}^{\alpha \dagger} \Sigma y_{E} = \delta_{22}$ while taking
$\Sigma E = L/(2\pi \hbar v_{F}) \int_{-\infty}^{+\infty} dE$, we arrive at a final answer for the total average current
at the first lead

$$I^1 = \frac{e}{4\hbar} \int_{-\infty}^{+\infty} dE \ f_{E}^{-1} \left\{ 2N^1 - 2 \Re[r_{E}^{1 \dagger} \tilde{r}_{22,E}^{1}] \right\}$$

$$- \text{Tr}[\Sigma y_{E}^{\alpha \dagger} \Sigma y_{E}^{\alpha}] \} \tag{2.7.19}$$

of which the part containing singular Majorana behavior as $\varphi$ goes through $\pi$ is

$$I_{\gamma} = -\frac{e}{2h} \int_{-\infty}^{+\infty} dE \ f_{-E}^{-1} \{ \Re[r_{E}^{1 \dagger} \tilde{r}_{22,E}^{1}] \}. \tag{2.7.20}$$

If we take the single-channel limit, i.e. the case of a quantum point contact,
$N^1 = N^2 = 1$ and $\tilde{r}_{E}^{\alpha}$ is reduced to $\tilde{r}_{22,E}^{1} = -\tilde{r}_{22,E}^{2} = 1$ and the average current
becomes

$$I^1 = \frac{e}{2h} \int_{-\infty}^{+\infty} dE \ f_{-E}^{-1} \left\{ 1 - \Re[r_{E}^{1 \dagger}] \right\} \tag{2.7.21}$$

In the more realistic many-channel limit, the elements of $\tilde{r}_{E}^{\alpha} \sim O(1/\sqrt{N^\alpha})$ but
with random phases. This means that they will, in general, not add coherently
such that in the large $N^\alpha$ limit, terms that contain $\tilde{r}_{E}^{\alpha}$ will die off. In this limit the
average current reads

\[ I_{\text{many}}^1 = \frac{e}{2\hbar} \int_{-\infty}^{+\infty} dE f_E^{-1} N^1, \]  

(2.7.22)

and the \( \varphi \) dependence is suppressed.

### 2.7.2 Cross Noise Calculation

In this section, we calculate in terms of our previous matrices the general expression for noise power, specializing at the end to the case of cross noise. Zero-frequency noise power, \( P^{\alpha\beta} = \int_{-\infty}^{+\infty} dt \left( \langle \hat{I}^\alpha(t) \hat{I}^\beta(0) \rangle - I^\alpha I^\beta \right) \), can be calculated using Wick’s theorem as follows:

\[
P^{\alpha\beta} = \frac{e^2 v_F}{L} \sum_{E,E'} \langle \gamma_{E'}^{a} \gamma_{E}^{c} \gamma_{E}^{d} \gamma_{E'}^{b} \rangle A_{E}^{a,b} A_{E'}^{c,d} \]

\[
= \frac{e^2 v_F}{L} \sum_{E} Q_{E}^{ac} Q_{E}^{bd} A_{E}^{a,b} A_{E}^{c,d} - \frac{e^2 v_F}{L} \sum_{E} Q_{E}^{ad} Q_{E}^{bc} A_{E}^{a,b} A_{E}^{c,d} \]

\[
= 2 \frac{e^2 v_F}{L} \sum_{E} \text{Tr}[A_{E}^{a} Q_{E}^{T} A_{E}^{b}] . \]  

(2.7.23)

From here, we can specialize to the \( \alpha \neq \beta \) case and calculate the cross noise power. For \( \alpha = 1, \beta = 2 \),

\[
P^{12} = 4 \frac{e^2 v_F}{L} \sum_{E} \text{Tr}[S_{E}^{x} S_{E}^{y} S_{E}^{z} Q_{E}^{1} S_{E}^{x} S_{E}^{y} S_{E}^{z} Q_{E}^{2} T] . \]

(2.7.24)

After specializing the S-matrix elements and taking \( \sum_{E} = (L/(2\pi \hbar v_F)) \int dE \), \( P^{12} \)
becomes

\[ P_{12}^{\gamma} = -\frac{e^2}{4\hbar} \int_{-\infty}^{+\infty} dE \frac{f_E^{-1} f_{E'}^{-1} t_E^1 t_{E'}^1 e_{12}^* e_{12}^{2*}}{t_{E'}^2}, \quad (2.7.25) \]

where we have used \( P_{12}^{\gamma} \) to note that all of \( P^{12} \) behaves singularly as the system goes through its critical point.

In the single-channel limit discussed in Appendix 2.7.1,

\[ P^{12} = \frac{e^2}{4\hbar} \int_{-\infty}^{+\infty} dE \frac{f_E^{-1} f_{E'}^{-1} t_E^1 t_{E'}^2}{t_{E'}^2}, \quad (2.7.26) \]

In the many-channel limit, \( P^{12} \to 0 \) as \( O(1/\sqrt{N_1 N_2}) \).

### 2.7.3 Diagonal Noise Calculation

The diagonal noise calculation follows very closely the cross noise calculation. However, unlike \( P^{12} \), \( P^{11} \) does not have a simple general form. We begin with Eq. (2.7.23)

\[ P^{11} = 2\frac{e^2 v_F}{L} \sum_E \text{Tr}[A_E^1 Q_{-E} A_E^1 Q_E^T], \quad (2.7.27) \]
which given Eq. (2.7.17) and (2.7.18) becomes

\[
P^{11} \equiv \frac{e^2}{8\hbar} \int_{-\infty}^{+\infty} dE \\
\left\{ \begin{array}{l}
 f_{-E}^{-1} f_{E}^{-1} \left\{ 4N^1 - 2 \text{Tr}[\Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1] - 2|t_E|^2 \right\} \\
 + f_{E}^{-1} f_{E}^{-1} \left\{ -2N^1 + 2 \text{Tr}[\Sigma_{y} \Sigma_{y}^1] \right\} \\
 - \text{Tr}[\Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1] \\
 + ( f_{E}^{-1} f_{E}^{+1} - f_{-E}^{-1} f_{E}^{+1} ) \left\{ 2 \text{Tr}[\Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1] \right\} \\
 + f_{E}^{-1} f_{E}^{+1} 2|t_E|^2 \right\} \quad (2.7.28)
\]

under the usual substitution for \( \Sigma_{E} \). Further simplifying this, we can obtain expressions for the traces of scattering matrices:

\[
\text{Tr}[\Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1] = |t_E|^2 (\tilde{r}_{E}^1 \Sigma_{y}^1)_{22}
\]

\[
\text{Tr}[\Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1] = 2 \text{Re}[r_{11}^1 \Sigma_{y}^1] + \text{Tr}[\Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1]
\]

\[
\text{Tr}[\Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1] = 2 \text{Re} \left[ (r_{-E}^1 \Sigma_{y}^1)_{22}^2 + r_{E}^1 (\tilde{r}_{E}^1 \Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1)_{22} \right] + \text{Tr}[\Sigma_{y} \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1 \Sigma_{y}^1]. \quad (2.7.29)
\]

This very complicated expression does not have, like the current and cross noise,
clearly separable singular pieces in its general N-channel form. However in the single-channel limit as described in Appendix 2.7.1, it simplifies significantly:

\[
P_{11} = \frac{e^2}{4\hbar} \int_{-\infty}^{+\infty} dE \left[ |1 - r_{E}^{1}|^2 f_{-E}^+ f_{E}^+ - (1 - r_{E}^{1})^2 f_{E}^- f_{-E}^- + |t_{E}|^2 f_{-E}^+ f_{E}^- \right], \tag{2.7.30}
\]

where we have exploited in the second term that \( f_{-E}^- = f_{E}^- \) and that \( r_{E}^{\alpha} = r_{E}^{\alpha_{*}} \).

In the many-channel limit, the diagonal noise becomes quite simple:

\[
P_{11}^{\text{many}} = \frac{e^2}{4\hbar} \int_{-\infty}^{+\infty} dE \ f_{E}^+ f_{-E}^+ \left\{ 2N^1 - |t_{E}|^2 \right\} + f_{E}^+ f_{-E}^+ |t_{E}|^2, \tag{2.7.31}
\]

where unlike with \( P_{12} \), the \( \varphi \) dependence is mostly preserved and is much more clearly extracted than in the general, N-channel case. Additionally, the singular part of the diagonal noise, \( P_{11}^{\gamma} \), goes to zero in the many-channel limit if \( V^1 = V^2 \).
Chapter 3

Critical Behavior of
Four-Terminal Conductance of
Bilayer Graphene Domain Walls

3.1 Abstract

Bilayer graphene in a perpendicular electric field can host domain walls between regions of reversed field direction or interlayer stacking. The gapless modes propagating along these domain walls, while not strictly topological, nevertheless have interesting physical properties, including valley-momentum locking. A junction where two domain walls intersect forms the analogue of a quantum point contact.
We study theoretically the critical behavior of this junction near the pinch-off transition, which is controlled by two separate classes of non-trivial quantum critical points. For strong interactions, the junction can host phases of unique charge and valley conductances. For weaker interactions, the low-temperature charge conductance can undergo one of two possible quantum phase transitions, each characterized by a specific critical exponent and a collapse to a universal scaling function, which we compute. *This chapter originally appeared as an article by Benjamin J. Wieder, Fan Zhang, and C. L. Kane in Physical Review B in 2015 [223].*

### 3.2 Introduction

#### 3.2.1 Background

Bilayer graphene [35, 144] provides an attractive platform for unconventional two-dimensional electronic physics due to the two quadratic band contacts at its Fermi points, and because of the variety of ways by which one can introduce a band gap and produce momentum-space Berry curvature [254]. The interlayer nearest-neighbor hopping, $\gamma_1$, warps the band structure of the individual graphene layers, repelling two bands away from the Fermi energy and leaving the remaining two dispersing quadratically. This warping is a consequence of the two-step process in which electrons hop between the two low-energy sublattices via the two high-energy ones. The band touching points at inequivalent Brillouin zone corners $K$ or $K'$ are pro-
ected by the Berry phase ±2π (or winding number ±2) and the required chiral (or
sublattice) symmetry between the low-energy sublattices on opposite layers [205].
Keeping all of these symmetries, the band touching point can only split, instead
of being gapped out, even when trigonal warping and other weak remote-hopping
processes are taken into account [144].

However, the chiral symmetry between the low-energy sublattices can be intrinsi-
cally broken by spin-orbit coupling [106], spontaneously broken by electron-electron
interactions [157, 253–255], or explicitly broken by an interlayer potential differ-
ence [144, 146, 161, 163]. As a consequence, the quadratic band touching is no
longer symmetry-protected and gaps open up at valleys $K$ and $K'$. While the first
two types of gaps are small in practice [17, 145, 205, 242], the electric-field-induced
gap, which is the focus of this chapter, saturates at a large value comparable to the
interlayer hopping $\gamma_1 \sim 0.3$ eV [146, 261]. Opening the band gap produces large
momentum-space Berry curvature in the quasiparticle bands, with the curvature
integral quantized to ±1 over a half Brillouin zone centered at $K$ or $K'$ [142, 254].
Moreover, for bilayer graphene gapped by an electric field, the sign of this partial
Chern number depends on the valley index, the sign of the energy gap (given by
the direction of interlayer electric field), and the layer stacking order (i.e., AB or
BA) [254, 257]. Here AB (BA) stacking refers to the case in which $\gamma_1$ couples the
top layer A (B) and bottom layer B (A) high-energy sublattices.

In the presence of an interlayer electric field, when the field direction is reversed
across a line [102, 124, 142, 172, 241, 250, 257] or when the field is uniform and the layer stacking switches from AB to BA [5, 204, 257], the valley-projected Chern number changes by 2 (−2) across the domain wall in valley $K$ ($K'$). As a result, both types of domain walls host two chiral edge states in each valley with chirality (direction) locked to valley index $K$ or $K'$, as shown in Fig. 3.1. Similar domain wall states also occur spontaneously due to interactions in the absence of electric fields but at finite temperature [127]. Importantly [257], these “Quantum Valley Hall” (QVH) edge states are not strictly topological and can be gapped out by a sufficiently strong, large-momentum scattering which couples the two valleys, even if the underlying symmetries are still preserved. It is therefore crucial that valley index also remains a “good quantum number,” for which we will assume that short-range disorder, interlayer stacking, and electric field direction changes are smooth on the scale of the lattice. Under this assumption, backscattering is prohibited and the system of domain walls provides an attractive platform for Tomonaga-Luttinger liquid physics [110].

In this chapter, we study the electronic transport properties of a junction where two domain walls intersect (Fig. 3.2). Such a structure resembles the quantum point contact of the edges of two Quantum Spin Hall (QSH) insulators, which has been studied in Refs. 91, 192, 199 and can be probed by four-terminal transport measurements. A domain wall junction can be tuned through a “pinch-off transition” by applying a local field (such as a perpendicular electric field) to the junction region. In Ref. 199, it was found that the corresponding pinch-off transition for QSH sys-
tems is controlled by a novel quantum critical point, and that at low temperatures the conductance is described by a universal scaling function across the pinch-off transition. In contrast to the QSH edge states, which have a single time-reversed pair of helical modes, the domain wall states in bilayer graphene host four helical pairs (including electron spin). We find that this leads to several important modifications of the low-energy properties of the junction.

Unlike with the QSH edge states, whose forward-scattering interactions are characterized by a single Luttinger parameter, it has been argued that for the domain wall states in bilayer graphene, one should characterize interactions with two independent Luttinger parameters [110]. This leads to an expanded phase diagram for the possible stable states of the junction. Moreover, we find that the pinch-off transition is modified. Depending on the interaction strengths, there are two possible regimes for the reduced, two-terminal conductance: one in which it undergoes a single pinch-off transition directly from 0 to $8e^2/h$ and one in which it undergoes two separate transitions, separated by a stable state with conductance $4e^2/h$. We study the critical behavior of these transitions and compute the universal crossover scaling functions for weak interactions.

This chapter is structured as follows. First we introduce in detail the domain wall states in bilayer graphene and derive low-energy effective field theories for them. Adding interactions, we show how these states are Luttinger liquids described by two independent Luttinger parameters. From there, we characterize the geometry
of two intersecting domain wall states in the language of the resulting effective quantum point contact. We then analyze the resulting four-terminal junction in both the context of many-body tunneling in a bosonization framework and with an S-matrix renomalization group using diagrammatic perturbation theory. Combining these analyses, we determine the behavior of the reduced, two-terminal conductance over a range of interaction strengths.

### 3.2.2 Measurable Results

In this chapter, we calculate several measurable properties of bilayer graphene domain wall quantum point contacts. In section 3.3.1, we find the critical exponent $\alpha_T$ which characterizes the low temperature tunneling conductance scaling for a single domain wall, a result previously derived in Ref. 110. In 3.3.2, we introduce a diagonal conductance $G_{ZZ} = 8e^2/h$, which is only strictly quantized when valley index is conserved both within individual domain walls and across the junction. This conductance, therefore, stands as a first test of whether experimental samples are in the appropriate disorder regime for the analysis in this chapter. We also show in 3.3.2 that states of exotic charge and valley tunneling character dominate the conductance of the junction under very strong attractive or repulsive interactions (Fig. 3.4). Finally, in 3.4.2.3, we show that the left-to-right conductance $G_{XX}$ undergoes either a direct transition from 0 to $8e^2/h$ or an indirect one with an intermediate step to $4e^2/h$ depending on experimental specifics (Fig. 3.9).
the direct transition $A$ and the first step of the indirect transition $B$, we go on to show that at low temperatures, the conductance transitions should collapse onto universal scaling functions $G_{A/B}$ with critical exponents $\alpha_{A/B}$ as functions of the interaction strengths (Figs. 3.10,3.11).

3.3 Model System

In this section we introduce our model system of bilayer graphene domain wall modes. First, we begin with the Hamiltonian for a single domain wall and the Luttinger liquid physics which govern it in the presence of interactions. Then, we discuss the four-terminal geometry which arises at the intersection of two domain walls and its equivalence to a quantum point contact.

3.3.1 Domain Walls in Bilayer Graphene

As discussed in the introduction, bilayer graphene domain walls can be created by varying the direction of the interlayer electric field or by varying the interlayer stacking order. In either case, The valley-projected Chern number changes by 2 ($-2$) across the domain wall in valley $K$ ($K'$). This necessitates the existence of two domain wall states in each valley, with the states at $K$ having equal and opposite velocities to those at $K'$. Adopting the notation of Ref. 110, we label these bands 0 and $\pi$ respectively (Fig. 3.1). For the purposes of our model, we will assume
Figure 3.1: Domain walls in bilayer graphene can be induced by applying a perpendicular electric field and varying either the interlayer stacking (a) or the electric field direction (b). Both kinds of domain walls (the dotted lines) have similar domain wall band structures (c) when the Fermi energy $E_F$ is near the chiral symmetric point. Adopting the notation of Ref. 110, the two domain wall states in each direction are labeled 0 and $\pi$ working from the Brillouin zone edge in. When the Fermi energy is exactly in the middle of the bulk gap, the Fermi velocities are the same for the 0 and $\pi$ bands and electron direction is set by valley index $K/K'$.
that the Fermi energy lies exactly in the middle of the bulk gap, which allows the simplification $v_{F,0} = v_{F,\pi} = v_F$. This allows us to write down the non-interacting Hamiltonian density

$$H_0 = i\hbar v_F \sum_{a=0,\pi} \sum_{\sigma=\uparrow,\downarrow} \psi_{a\sigma,in}^{\dagger} \partial_x \psi_{a\sigma,in} - \psi_{a\sigma,out}^{\dagger} \partial_x \psi_{a\sigma,out}$$  

(3.3.1)

where the indexes “in” and “out” refer to direction and can correspond to electron operators with valley index $K$ or $K'$ depending on the orientation of the domain wall. We will see later that in a four-terminal structure, the correspondence between in/out and $K/K'$ will alternate with lead index due to the valley-momentum locking of the domain wall modes.

In the limit of the Fermi energy resting exactly at the chiral-symmetric point, the band indexes become arbitrary labels for all of the calculations in this chapter. A consequence of this is the emergence of a band-index-exchange symmetry in this problem, which we will frequently highlight in calculations throughout this chapter. Deviations from this point in the Fermi energy are expected in physical systems, and will lead in general to a relaxation of this symmetry. If the deviations are small, the physics should resemble the predictions of this chapter, with corrections of order $\sim 1 - v_{F,0}/v_{F,\pi}$. These corrections greatly complicate the calculations in this chapter and obscure key generalities, and to that end we consider $v_{F,0} = v_{F,\pi} = v_F$ a desirable simplification of this problem.
Calculations by Killi, Wei, Affleck, and Paramekanti indicated that for interacting bilayer graphene systems, the interaction is dominated by two density-density interactions [110]:

\[
V_+ = u_+(n_{0\uparrow} + n_{0\downarrow} + n_{\pi\uparrow} + n_{\pi\downarrow})^2
\]

\[
V_- = u_-(n_{0\uparrow} + n_{0\downarrow} - n_{\pi\uparrow} - n_{\pi\downarrow})^2.
\]  

(3.3.2)

\[V_+\] is the usual two-body forward scattering term which leads to Luttinger liquid physics and \[V_-\] is a new one which breaks the \(U(2)\) symmetry of electron distribution between the 0 and \(\pi\) bands. Both can be effectively tuned by altering the strength of the perpendicular electric field, though for all reasonable numerical estimates, Ref. 110 found \(u_- < u_+\) and \(u_-\) harder to tune, which is sensible as only \(V_+\) contains contributions from the long-range part of the Coulomb interaction.

Other density-density interactions, specifically those which affect electron spin, should be small in practice. In the absence of an external magnetic field, and given the weak spin-orbit interaction in graphene, electron spin should remain SU(2)-symmetric. In this limit, the electron spin sectors of this problem should remain noninteracting and terms which lead to phenomena such as spin-density waves will be marginally irrelevant [71].
Returning to our Hamiltonian, we can consider a single domain wall by bosonizing,

\[ \psi_{a\sigma,i} = \frac{1}{\sqrt{2\pi x_c}} e^{i\phi_{a\sigma,i}} \]  

(3.3.3)

where \( a = 0, \pi; \sigma = \uparrow, \downarrow; i = \text{in, out} \) and \( x_c \) is the short wavelength cutoff. The bosonic fields \( \phi_{a\sigma,i} \) obey the commutation algebra:

\[ [\phi_{a\sigma,i}(x), \phi_{b\sigma',j}(y)] = i\pi \delta_{ab} \delta_{\sigma\sigma'} \tau_{ij}^z \text{sgn}(x - y). \]  

(3.3.4)

Under this transformation, the bare Hamiltonian and interactions become:

\[ \mathcal{H}_0 = \frac{\hbar v_F}{4\pi} \sum_{\sigma=\uparrow,\downarrow} \left[ (\partial_x \phi_{0\sigma,\text{in}})^2 + (\partial_x \phi_{0\sigma,\text{out}})^2 \right. \]
\[ + \left. (\partial_x \phi_{\pi\sigma,\text{in}})^2 + (\partial_x \phi_{\pi\sigma,\text{out}})^2 \right] \]
\[ V_{\pm} = \frac{\hbar v_F}{8\pi} \lambda_{\pm} \sum_{\sigma=\uparrow,\downarrow} \left[ (\partial_x \phi_{0\sigma,\text{in}} - \partial_x \phi_{0\sigma,\text{out}})^2 \right. \]
\[ + \left. (\partial_x \phi_{\pi\sigma,\text{in}} - \partial_x \phi_{\pi\sigma,\text{out}})^2 \right] \]  

(3.3.5)

where \( \lambda_{\pm} = \frac{u_{\pm}}{\pi \hbar v_F} \). The interacting Hamiltonian can be simplified by the sum/difference changes of basis:
\[ \phi_{\pm\sigma,i} = \phi_{0\sigma,i} \pm \phi_{\pi\sigma,i} \]
\[ \phi_{\pm c/s,i} = \phi_{\pm\uparrow,i} \pm \phi_{\pm\downarrow,i} \]  \hspace{1cm} (3.3.6)

where the \( c \) and \( s \) sectors are charge and spin respectively. In this basis, all of the interactions are in the charge sector and, as motivated earlier in this section, the spin sector is noninteracting:

\[ H_0 = H_+ + H_- + H_s + H_{s} \]
\[ H_{\pm c/s} = \frac{\hbar v_F}{8\pi} \left[ (\partial_x \phi_{\pm c/s,in})^2 + (\partial_x \phi_{\pm c/s,out})^2 \right] \]
\[ V_{\pm} = \frac{\hbar v_F}{8\pi} \lambda_{\pm c} \left[ \partial_x \phi_{\pm c,in} - \partial_x \phi_{\pm c,out} \right]^2. \]  \hspace{1cm} (3.3.7)

The plus and minus charge sectors of \( H_0 \) are then each renormalized by only \( V_{\pm}\) respectively, encouraging us to express the interaction parameter \( g_{\pm}\) separately for each charge sector.

Therefore we can write down the interacting Hamiltonian for each charge sector, \( H_{\pm c,int} = H_{\pm c} + V_{\pm} \). Diagonalizing this Hamiltonian, the definition of the Luttinger parameters \( g_{\pm}\) arises naturally. The change of basis
\[
\begin{pmatrix}
\phi_{\pm c,\text{in}} \\
\phi_{\pm c,\text{out}}
\end{pmatrix} = \frac{1}{2g_{\pm}} \begin{pmatrix}
1 + g_{\pm} & 1 - g_{\pm} \\
1 - g_{\pm} & 1 + g_{\pm}
\end{pmatrix} \begin{pmatrix}
\tilde{\phi}_{\pm c,\text{in}} \\
\tilde{\phi}_{\pm c,\text{out}}
\end{pmatrix}
\] (3.3.8)

returns our interacting Hamiltonian to the form of one for non-interacting chiral bosons

\[
H_{\text{int}} = H_{+c,\text{int}} + H_{-c,\text{int}} + H_{+s} + H_{-s}
\]

\[
H_{\pm c,\text{int}} = \frac{\hbar v_{\pm}}{8\pi g_{\pm}} \left[ (\partial_x\tilde{\phi}_{\pm c,\text{in}})^2 + (\partial_x\tilde{\phi}_{\pm c,\text{out}})^2 \right]
\] (3.3.9)

where

\[
v_{\pm} = v_F \sqrt{1 + 2\lambda_{\pm}}, \quad g_{\pm} = \frac{1}{\sqrt{1 + 2\lambda_{\pm}}}. \quad (3.3.10)
\]

In the new basis, the charge fields \( \tilde{\phi}_{\pm c,i} \) obey the commutation relation:

\[
\left[ \tilde{\phi}_{uc,i}(x), \tilde{\phi}_{vc,j}(y) \right] = i\pi g_u \delta_{uv} \tau_{ij}^z \text{sgn}(x - y)
\] (3.3.11)

where \( u, v = +, -; \ i = \text{in, out} \); and we note that the noninteracting spin sector fields still obey this commutation relation with \( g_{\pm} = 1 \).
As in Refs. 91, 192, 199, the tunneling density of states for a single edge $\rho(E) \propto E^{\alpha_T}$ is controlled by the interactions. However here, unlike in the QSH case, the critical exponent is a function of two Luttinger parameters, such that in agreement with Ref. 110,

$$\alpha_T = \frac{1}{8} (g_+ + g_- + 1/g_+ + 1/g_-) - \frac{1}{2},$$  \hfill (3.3.12)

From an experimental perspective, measuring this critical exponent for the tunneling conductance would be a valuable first step in confirming the Luttinger liquid physics of these bilayer graphene domain wall states.

### 3.3.2 Four-Terminal Geometry

A pattern of two domain walls which pass nearly by each other can be formed by varying either electric field direction or interlayer stacking twice (Fig. 3.2a). If we distort the central region of this picture, we could imagine bringing the two domain walls so close that tunneling between them becomes significant. In this case, the two domain walls have formed the equivalent of a quantum point contact (Fig. 3.2b). Mapping our work in 3.3.1 onto a spinful Luttinger liquid for the two-wall system, we deduce in this section, for all interaction regimes, the interaction strengths at which many-body tunneling processes become relevant and alter the junction’s charge and valley conductances.
Figure 3.2: (a) Two parallel domain walls in bilayer graphene can be created by varying either the interlayer stacking or the perpendicular field direction between regions A and B. (b) Distorting region B such that the walls approach each other results in the equivalent of a Quantum Point Contact (QPC) for the domain wall modes. The numbers 1 – 4 are lead indexes and the two modes displayed for each domain wall are those at 0 and at $\pi$. All of the modes shown here are at valley $K$; a counterpropagating set of modes exists at $K'$ and is related by time-reversal symmetry. Including electron spin, there are 4 modes in each valley in each domain wall, for a total of 16 modes to consider for this QPC structure.

While each lead retains the properties and Luttinger parameters from 3.3 individually, we will find it convenient to limit the usage of the $\tilde{\varphi}_\pm$ basis to the treatment of isolated domain walls and adopt a new basis with effective charge and valley sectors. The charge sector which arises here is a new degree of freedom and comes from a rotation of the indexes for $K$ and $K'$ and propagation direction. We will label these charge and valley sectors $\rho$ and $\nu$ respectively to differentiate them from the charge and spin sectors which arose in 3.3.1, which are labeled $c$ and $s$ respectively.

The two domain walls in Fig. 3.2 have opposite helicities, due to being on the top (bottom) of the central region. We can define, for the interacting system, fields labeled by sum/difference, charge/spin, direction, and valley $(K, K')$: 

```plaintext
Figure 3.2: (a) Two parallel domain walls in bilayer graphene can be created by varying either the interlayer stacking or the perpendicular field direction between regions A and B. (b) Distorting region B such that the walls approach each other results in the equivalent of a Quantum Point Contact (QPC) for the domain wall modes. The numbers 1 – 4 are lead indexes and the two modes displayed for each domain wall are those at 0 and at $\pi$. All of the modes shown here are at valley $K$; a counterpropagating set of modes exists at $K'$ and is related by time-reversal symmetry. Including electron spin, there are 4 modes in each valley in each domain wall, for a total of 16 modes to consider for this QPC structure.

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The two domain walls in Fig. 3.2 have opposite helicities, due to being on the top (bottom) of the central region. We can define, for the interacting system, fields labeled by sum/difference, charge/spin, direction, and valley $(K, K')$: 

```
\[\begin{align*}
\phi_{\pm c/s,RK} &= \phi_{\pm c/s,in,1}(-x)\Theta(-x) + \phi_{\pm c/s,out,2}(x)\Theta(x) \\
\phi_{\pm c/s,LK'} &= \phi_{\pm c/s,out,1}(-x)\Theta(-x) + \phi_{\pm c/s,in,2}(x)\Theta(x) \\
\phi_{\pm c/s,LK} &= \phi_{\pm c/s,in,3}(x)\Theta(x) + \phi_{\pm c/s,out,4}(-x)\Theta(-x) \\
\phi_{\pm c/s,RK'} &= \phi_{\pm c/s,out,3}(x)\Theta(x) + \phi_{\pm c/s,in,4}(-x)\Theta(-x)
\end{align*}\]

where \(\Theta(x)\) is the Heaviside step function and the indexes 1 \(- 4\) on the noninteracting \(\phi_{\pm}\) refer to the individual lead in Figure 3.2 with which they are associated.

The intersection of the two domain walls occurs at \(x = 0\) such that our theory consists of four, isolated domain walls everywhere except at that point. Assuming that the interaction strength is controlled globally such that each lead has the same values of \(\lambda_{\pm}\), we can create a \(\rho/v\) basis for each +/- sector of the combined Hamiltonian of the two domain walls \(\mathcal{H}_{int} = \sum_{i=1}^{4} \sum_{\alpha=c,s}(\mathcal{H}_{\alpha,int}^i + \mathcal{H}_{-\alpha,int}^i)\):
\[
\phi_{\pm c/s, RK} = \frac{1}{2} \left[ \phi_{\pm c/s, \rho} + \phi_{\pm c/s, v} + \theta_{\pm c/s, \rho} + \theta_{\pm c/s, v} \right]
\]
\[
\phi_{\pm c/s, LK} = \frac{1}{2} \left[ \phi_{\pm c/s, \rho} + \phi_{\pm c/s, v} - \theta_{\pm c/s, \rho} - \theta_{\pm c/s, v} \right]
\]
\[
\phi_{\pm c/s, RK'} = \frac{1}{2} \left[ \phi_{\pm c/s, \rho} - \phi_{\pm c/s, v} + \theta_{\pm c/s, \rho} - \theta_{\pm c/s, v} \right]
\]
\[
\phi_{\pm c/s, LK'} = \frac{1}{2} \left[ \phi_{\pm c/s, \rho} - \phi_{\pm c/s, v} - \theta_{\pm c/s, \rho} + \theta_{\pm c/s, v} \right]
\]

(3.3.14)

where again \(c, s\) are the charge and spin sectors which resulted from rotating the indexes for \(\uparrow, \downarrow\) and \(\rho, v\) are the indexes which have, along with the choice of \(\phi, \theta\), resulted from rotating indexes for propagation direction \((R, L)\) and valley \((K, K')\).

The new fields are governed by the modified commutation relation:

\[
[\theta_{u\alpha i}(x), \phi_{v\beta j}(y)] = 2\pi i \delta_{uv} \delta_{\alpha\beta} \delta_{ij} \Theta(x - y)
\]

(3.3.15)

where \(u, v = +, -; \alpha, \beta = c, s\); and \(i, j = \rho, v\).

This unitary rotation of the variables effectively changes the sign of the interaction “cross-term” individually for the choice of \(\phi, \theta, \rho, v\) within the \(c\) sector:
\[ H_{\pm,\text{int}} = \frac{\hbar v_F}{8\pi} \left\{ (1 + \lambda_\pm) \left[ (\partial_x \phi_{\pm cp})^2 + (\partial_x \phi_{\pm cv})^2 \right] + (\partial_x \theta_{\pm cp})^2 + (\partial_x \theta_{\pm cv})^2 \right\} - \lambda_\pm \left[ (\partial_x \phi_{\pm cp})(\partial_x \phi_{\pm cp}) - (\partial_x \phi_{\pm cv})(\partial_x \phi_{\pm cv}) \right] \]
\[ - (\partial_x \theta_{\pm cp})(\partial_x \theta_{\pm cp}) + (\partial_x \theta_{\pm cv})(\partial_x \theta_{\pm cv}) \} \].

(3.3.16)

The previous equation, though diagonal, was left unsimplified and in the form of Eq. 3.3.5 such that by the same logic as in 3.3.1, the form of the simplified diagonalized Hamiltonian, as well as the interactions, can just be read off:

\[ H_{\pm,\text{int}} = \frac{\hbar v_\pm}{8\pi} \sum_{\alpha = c,s} \sum_{a = \rho,\nu} g_{\pm \alpha a} (\partial_x \phi_{\pm \alpha a})^2 + \frac{1}{g_{\pm \alpha a}} (\partial_x \theta_{\pm \alpha a})^2 \]
\[ g_{\pm cp} = g_\pm, \quad g_{\pm cv} = 1/g_\pm, \quad g_{\pm \rho} = g_{\pm \nu} = 1 \]  

(3.3.17)

such that \( H_{\text{int}} \) now has the form of a spinful Luttinger liquid. In this basis, both the interacting and noninteracting Hamiltonians are diagonal and so the transformation between the interacting and noninteracting \( \theta/\phi \) requires just a simple rescaling by the interaction parameter for each sector.
For this geometry, one can probe experimentally by measuring the current $I_i$ at one of the leads in response to an applied voltage on another lead $V_j$ such that a $4 \times 4$ conductance matrix characterizes the system,

$$I_i = G_{ij} V_j \quad (3.3.18)$$

where $i = 1 - 4$ is a lead index. In the presence of time-reversal and valley symmetries, the number of independent or nonzero parameters in $G_{ij}$ is greatly reduced, as described in detail in the appendix of Ref. 199. For this system, we can then consider a reduced set of voltages and currents:

$$\begin{pmatrix}
  I_X \\
  I_Y
\end{pmatrix} =
\begin{pmatrix}
  G_{XX} & G_{XY} \\
  G_{YX} & G_{YY}
\end{pmatrix}
\begin{pmatrix}
  V_X \\
  V_Y
\end{pmatrix} \quad (3.3.19)$$

where $I_X = I_1 + I_4$ is the left-to-right current and $I_Y = I_1 + I_2$ is the top-to-bottom current. $V_X$ and $V_Y$ are similarly defined such that $V_X$ is a bias of leads 1 and 4 relative to leads 2 and 3 and $V_Y$ is a bias of leads 1 and 2 relative to leads 3 and 4. Therefore $G_{XX}$ and $G_{YY}$ are the two-terminal conductances measured left-to-right and top-to-bottom respectively. $G_{XY} = G_{YX}$ are skew conductances, equal as a consequence of time-reversal symmetry. In the noninteracting model, this skew conductance is zero as a consequence of artificial spatial symmetries, such as mirror symmetry. Though it may become nonzero under increased interaction
strengths, the skew conductance is still negligible along the relevant directions which characterize transitions in this system [199]. We can define a final current across the junction $I_Z = I_1 + I_3$, which one can probe by applying a voltage $V_Z$ which biases leads 1 and 3 relative to leads 2 and 4, with a conductance

$$I_Z = G_{ZZ} V_Z. \quad (3.3.20)$$

If valley is conserved, then electrons cannot enter at lead 1 and exit at lead 3, implying that a measurement of an exactly quantized

$$G_{ZZ} = \frac{8e^2}{h} \quad (3.3.21)$$

would be an experimental confirmation that valley-nonconserving disorder is absent and the system is appropriately described by the physics in this chapter. The factor of $N = 8$ in the Landauer prediction $G = Ne^2/h$ comes from factors of 2 for band index (0 and $\pi$), electron spin degeneracy, and the two incoming leads at $K$ (1 and 3).

We can also, in a similar manner, characterize the valley conductance of the system in terms of left-to-right and top-to-bottom parameters $G_{XX}^V$ and $G_{YY}^V$. Before the introduction of any interactions or tunneling operators, our system consists of two, left-to-right domain wall states and we consider it “fully-open.” For this sys-
Figure 3.3: Schematic of the valley-preserving single-particle tunneling processes. Many-body processes which conserve spin and valley can be constructed as products of these processes. Among the processes which conserve valley, only spin-conserving processes can become relevant and destabilize the fully pinched-off II (t) and fully-open (v) CC phases, due to the nature of the scaling dimension calculation. For each process about the charge and valley conducting phase (a), there is a dual process about the charge and valley insulating phase (b). The diagram here depicts modes for only a single spin direction; the full QPC hosts an additional set of modes related by a spin flip.

\[ G_{XX} = \frac{8e^2}{h} \text{ and } G_{XX}^V \neq 0 \] such that it is a left-to-right charge conductor, valley conductor, which we will denote as the CC phase. A 90° rotation and relabeling (with regards to Fig. 3.2) or the pinch-off inversion of this phase, for which \( G_{XX} = G_{XX}^V = 0 \text{ and } G_{YY} = \frac{8e^2}{h}, G_{YY}^V \neq 0 \), is considered “fully pinched-off” and is a left-to-right charge insulator, valley insulator, which we denote as the II phase.

With this framework established, we can examine perturbatively tunneling processes between the two adjacent domain walls which may lead to differing charge and valley conductances. Using our bosonization work, we can examine the rescaling of the coupling strength for each process, noting the interaction regime in which it dominates the physics of the quantum point contact.
Figure 3.3 illustrates the single-particle valley-conserving processes which can exist in this system within a single spin channel. In general, many-body tunneling processes will also be present and may become relevant. These many-body tunneling processes can be considered products of single-electron-tunneling processes which, in the most general case, may or may not conserve spin or valley indexes. However, restricting ourselves to the set of processes which conserve valley, it becomes apparent that the linear combinations of bosonized operators which can lead to relevant operators can only be achieved through products of single-particle processes which conserve spin. Therefore, in the analysis of many-body processes which may become relevant and drive to phases with different conductance behavior, we can simply consider products of spin- and valley-conserving single-electron tunneling:

\[ O_{\sigma u}^{\alpha \beta} = \psi_{\alpha \sigma R u}^{\dagger} \psi_{\beta \sigma L u}, \quad V_{n-\text{body}} = v_n \prod_{i=1}^{n} O_i + H.C. \]  

(3.3.22)

where \( \alpha, \beta = 0, \pi; \sigma = \uparrow, \downarrow; u = K, K'; v_n \) is the coupling strength of the process; and \( O_i \) is an arbitrary valley- and spin-conserving single-particle tunneling process. For the sake of condensing notation, tunneling from \( \beta, L \rightarrow R, \alpha \) will be expressed as \( O_{\sigma u}^{\alpha \beta \dagger} \). Weak tunneling about the CC phase (Fig. 3.3a) is related to weak backscattering in the left-to-right direction, and is also dual to weak tunneling about the II phase (Fig. 3.3b). Taking advantage of this duality, we will restrict our discussion to the set of \( v \) operators which may destabilize the CC phase, noting that the \( t \) tunneling operators about the II phase are related by a duality. This
Figure 3.4: The regions in interaction space for which tunneling processes become relevant ($\Delta < 1$ in Eqs. (3.3.28) and (3.3.30)) and the fully open (CC) or pinched-off (II) junction phases are destabilized. The central dot at $g_+ = g_- = 1$ is the noninteracting point and the dotted oval is the region of predicted accessible interaction strength in Ref. 110 for a suspended sample. The IC (CI) regions are characterized by four-body tunneling processes which transmit exclusively valley (charge) across the junction. The B regions represent relevant eight-body tunneling processes which are charge insulating (+) or conducting (−) and differ by band-index and valley-transmission character. Regions of overlap between boundaries, denoted with *, have multiple relevant operators at different orders and presumably more complicated behavior. In the central region, the fully open (CC) or pinched-off (II) phases remain stable and the conductance is characterized by single-electron tunneling.

duality is explored in greater detail in Ref. 199.

The near-intersection of the two domain walls is a $0+1$-dimensional object, and therefore the coupling strength $v_a$ of a given tunneling process flows, to first order, as

$$\frac{dv_a}{dl} = (1 - \Delta(v_a))v_a$$

(3.3.23)

where $\Delta(v_a)$ is the scaling dimension of the tunneling process $V_a$. 

84
To understand which operators may become relevant, we can first examine the single-electron tunneling processes (Fig. 3.3a):

\[ V_1 = v_1 \sum_{\alpha\beta,\sigma,u} O_{\alpha\beta}^{\alpha\beta} + H.C. \]  

(3.3.24)

where \( \alpha, \beta = 0, \pi; \sigma = \uparrow, \downarrow; u = K, K'; \) and we have restricted ourselves to processes which preserve spin and valley.

For single-particle tunneling,

\[ \Delta(v_1) = \frac{1}{8} \left[ g_+ + \frac{1}{g_+} + g_- + \frac{1}{g_-} + 4 \right] \]  

(3.3.25)

such that single-electron tunneling is always marginal or irrelevant (\( \Delta(v_1) \geq 1 \)) for all possible inter- and intra-band scattering processes. In the nearly noninteracting regime, where the least irrelevant operators are \( V_1 \), the strength of \( v_1 \) can be controlled by an external parameter, such as the gate voltage \( V_G \) for a given set of interaction strengths \( g_{\pm} \). In this interaction regime, we know that the CC and II phases are stable and that at least one quantum critical point exists to mediate the transition between them. In the subsequent section, Section 3.4, we will use diagrammatic perturbation theory in the interactions about the CC phase to search for the set of possible intermediate phases and quantum critical points which characterize the single-electron-tunneling behavior of the junction.
The factor of $4/8$ in $\Delta(v_1)$ is due to $g_{\pm spin} = g_{\pm valley} = 1$ and will remain an obstacle to a process becoming relevant unless the operator in bosonized form only contains $c$-sector variables. For higher-body tunneling, this factor is greater than or equal to 1, and prevents any process which isn’t pairwise spin conserving and invariant under arbitrary SU(2) spin rotations from becoming relevant. One can view this as pairwise spin conservation allowing decomposition into products of $O_{\sigma \alpha \beta}$ and SU(2) invariance providing the necessary linear combinations of $\sigma = \uparrow, \downarrow$ to isolate $c$ sector variables. Restricting to processes which conserve valley and obey these spin index constraints, the first operators to become relevant as interactions are increased are therefore a specific set of four- and eight-body tunneling processes.

Figure 3.4 details the region in interaction space for which each class of many-body operators becomes relevant ($\Delta(v_a) < 1$). When a process becomes relevant, the bosonized operators will become locked into the values which minimize the tunneling operator and become gapped out, altering the conductance of the junction. As an applied voltage only couples to the total electron density, only relevant operators containing $\theta_{+ spin}$ or $\phi_{+ spin}$ can cause the junction to become charge insulating. In the central region, all operators are marginal or irrelevant, though single-electron tunneling $V_1$ is only the least irrelevant operator close to the non-interacting point $g_+ = g_- = 1$.

Four groups of four-body processes are present which can become relevant and drive to phases which are completely charge or valley insulating:
\[
V_{IA} = v_{IA}^{(1)} \left[ O^{00}_{\uparrow K} O^{00}_{\uparrow K'} O^{00}_{\downarrow K} O^{00}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \\
+ v_{IA}^{(2)} \left[ O^{0\pi}_{\uparrow K} O^{\pi 0}_{\uparrow K'} O^{0\pi}_{\downarrow K} O^{\pi 0}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \quad + H.C.
\]

\[
V_{IB} = v_{IB}^{(1)} \left[ O^{00}_{\uparrow K} O^{\pi 0}_{\uparrow K'} O^{00}_{\downarrow K} O^{\pi 0}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \\
+ v_{IB}^{(2)} \left[ O^{0\pi}_{\uparrow K} O^{0\pi}_{\uparrow K'} O^{0\pi}_{\downarrow K} O^{0\pi}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \quad + H.C.
\]

\[
V_{IA} = v_{IA}^{(1)} \left[ O^{00}_{\uparrow K} O^{00\dagger}_{\uparrow K'} O^{00\dagger}_{\downarrow K} O^{00}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \\
+ v_{IA}^{(2)} \left[ O^{0\pi}_{\uparrow K} O^{\pi 0\dagger}_{\uparrow K'} O^{0\pi\dagger}_{\downarrow K} O^{0\pi}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \quad + H.C.
\]

\[
V_{IB} = v_{IB}^{(1)} \left[ O^{\pi\pi}_{\uparrow K} O^{\pi\pi\dagger}_{\uparrow K'} O^{\pi\pi\dagger}_{\downarrow K} O^{\pi\pi}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \\
+ v_{IB}^{(2)} \left[ O^{0\pi}_{\uparrow K} O^{0\pi\dagger}_{\uparrow K'} O^{0\pi\dagger}_{\downarrow K} O^{0\pi}_{\downarrow K'} + 0 \leftrightarrow \pi \right] \quad + H.C.
\]

or in bosonized form:

(3.3.26)
\[ V_{IC_A} = \cos(\theta_{+cp}) \left[ v_{IC_A}^{(1)} \cos(\theta_{-cp}) + v_{IC_A}^{(2)} \cos(\phi_{-cp}) \right] \]
\[ V_{IC_B} = \cos(\theta_{+cp}) \left[ v_{IC_B}^{(1)} \cos(\theta_{-cv}) + v_{IC_B}^{(2)} \cos(\phi_{-cp}) \right] \]
\[ V_{CI_A} = \cos(\theta_{+cv}) \left[ v_{CI_A}^{(1)} \cos(\theta_{-cv}) + v_{CI_A}^{(2)} \cos(\phi_{-cv}) \right] \]
\[ V_{CI_B} = \cos(\theta_{+cv}) \left[ v_{CI_B}^{(1)} \cos(\theta_{-cv}) + v_{CI_B}^{(2)} \cos(\phi_{-cv}) \right] \]

(3.3.27)

where \( v_{IC/CI}^{(1/2)} \) are the coupling constant strengths for the two different choices of interband scattering for each class of tunneling process and have absorbed factors of 2 during bosonization and simplification. The scaling dimensions for these couplings strengths are:
\[
\Delta(v_{IC_A}^{(1)}) = \Delta(v_{IC_A}^{(2)}) = 2g_+ + 2g_-
\]

\[
\Delta(v_{IC_B}^{(1)}) = \Delta(v_{IC_B}^{(2)}) = 2g_+ + \frac{2}{g_-}
\]

\[
\Delta(v_{CI_A}^{(1)}) = \Delta(v_{CI_A}^{(2)}) = \frac{2}{g_+} + 2g_-
\]

\[
\Delta(v_{CI_B}^{(1)}) = \Delta(v_{CI_B}^{(2)}) = \frac{2}{g_+} + 2g_-
\]

In the regions where the IC (CI) operators become relevant, the system will be charge (valley) insulating and valley (charge) conducting. Expressed in terms of conductance elements, the IC (CI) phases will have \(G_X = G_Y = 0\), \(G_{XX}^V = G_{YY}^V \neq 0\) (\(G_X = G_Y = 8e^2/h\), \(G_{XX}^V = G_{YY}^V = 0\)). These phases are related to the charge and spin insulating phases for the topological insulator QPC [199]. However, unlike those phases, the IC and CI phases in the bilayer graphene junction will still be transmitting in the spin sector as long as \(g_{\pm sp/v}\) are relatively close to noninteracting.

The remainder of the II/CC region is bounded by four eight-body processes. Each one can be considered as a product of one of the terms in the previous four-
body processes multiplied by a product of selected conjugates of itself as to isolate just a single charge-sector variable. In bosonized variables, these eight-body tunneling operators are:

\[ V_{B_i}^\pm = v_{B_i}^{(1)} \cos(2\theta_{\pm c\rho}) + v_{B_i}^{(2)} \cos(2\phi_{\pm c\nu}) \]
\[ V_{B_2}^\pm = v_{B_2}^{(1)} \cos(2\theta_{\pm c\nu}) + v_{B_2}^{(2)} \cos(2\phi_{\pm c\rho}) \] (3.3.29)

The strengths of these operators have scaling dimensions:

\[ \Delta(v_{B_i}^{(1)}) = \Delta(v_{B_i}^{(2)}) = 8g_{\pm} \]
\[ \Delta(v_{B_2}^{(1)}) = \Delta(v_{B_2}^{(2)}) = \frac{8}{g_{\pm}} \] (3.3.30)

They are only relevant under extremely strong interactions \((g_{\pm} < 1/8 \text{ or } g_{\pm} > 8)\) and are charge insulating (+) or conducting (−).

Higher-order many-body tunneling processes are of course also possibly relevant, however due to the nature of the scaling dimension calculation, they will become relevant at much larger values of interaction strength than the boundaries of the shaded regions in Figure 3.4.
3.4 The Pinch-Off Transition

As demonstrated in the previous section, under weak interactions the junction is stable in either the open (CC) phase or the closed-off (II) phase, both of which are characterized by single-electron tunneling and are related to each other by both 90° rotations and the pinch-off duality. In this section, we expand perturbatively in the interactions about the CC fixed point in search of the quantum critical point(s) which characterize the CC↔II quantum phase transition. In the process, we discover that, in addition to the $T_{0/\pi} = 1/2$ critical point, which is expected as a consequence of the pinch-off duality, an additional family of intermediate critical points and phases are also present. For each of the possible paths between the II and CC phases we derive the conductance signatures which characterize the low-temperature transitions as functions of the two interaction strengths and the external gate voltage. First, we show how the general S-matrix characterizing the junction is renormalized by weak interactions, deriving a phase diagram and Renormalization Group (RG) in the case where scattering between the 0 and $\pi$ bands is disallowed. We then allow for interband scattering, as might be present in the case of relatively smooth disorder, and introduce an S-matrix parameterization incorporating the additional system parameters. Using the results of an extensive renormalization group calculation, detailed in Appendix 3.7.1, we assert that the most general S-matrix flows back to one with small-momentum conservation. The RG flow on this surface therefore contains all of the characteristic non-trivial quan-
tum critical points for the pinch-off transition of this problem. Finally, we derive the
critical exponents and universal scaling functions for the two classes of conductance
transitions, up to leading order in the interactions.

3.4.1 Non-Interacting Electrons

In the absence of interactions, tunneling through the junction can be character-
ized by an S-matrix restricted only by time-reversal symmetry and valley-index
conservation

$$|\psi_{i,\text{out}}^{\alpha\sigma}\rangle = S_{ij}^{\alpha\beta}\delta^{\sigma\sigma'}|\psi_{j,\text{in}}^{\beta\sigma'}\rangle$$  \hspace{1cm} (3.4.1)

where $i, j$ are lead indexes 1 – 4; $\sigma, \sigma'$ are spin indexes $\uparrow, \downarrow$; and $\alpha, \beta$ are band
indexes 0 and $\pi$. Given the negligible spin-orbit coupling in graphene, we can con-
sider here that the time-reversal operator $\mathcal{T} = K$ leaves the spin sector unaffected,
such that $\mathcal{T}^2 = +1$. Therefore, time-reversal symmetry restricts that $S_{ij}^{\alpha\beta} = S_{ji}^{\beta\alpha}$. Additionally, to keep the domain wall states gapless, one must disallow scattering
from $K$ to $K'$, which restricts elements of the S-matrix $S_K = S_{K'}^T$. In this section,
we will work the most general allowed S-matrix down to one which is characterized
by parameters which have physical meaning. Beginning with the modes in a single
valley $K$:
where the rows and columns of $S_K$ indicate scattering of the incoming modes with valley index $K$ (leads 1 and 3) to the outgoing ones (leads 2 and 4). The matrices $\mathbb{r}$ and $\mathbb{l}$ live in the $2 \times 2$ space of band indexes. Identical copies of $S_K$ exist for the up and down spins. The elements of $S_K$ are otherwise unconstrained if we allow scattering between the 0 and $\pi$ bands such that $S_K$ is an arbitrary $U(4)$ matrix. We can choose to parameterize

$$S_K = \begin{pmatrix} \mathbb{l} & \mathbb{r} \\ -\mathbb{r}^\dagger & \mathbb{l}^\dagger \end{pmatrix}$$

(3.4.2)

$$t = \begin{pmatrix} \sqrt{T_0} & 0 \\ 0 & \sqrt{T_\pi} \end{pmatrix}, \quad r = \begin{pmatrix} \sqrt{1 - T_0^2} & 0 \\ 0 & \sqrt{1 - T_\pi^2} \end{pmatrix}$$

(3.4.3)

where the $U_i$ ($U_j^\dagger$) are for now unconstrained $U(2)$ matrices which characterize operations on the outgoing (incoming) electronic wavefunction at lead $i$ ($j$) and valley index $K$. In this parameterization, we can choose the tunneling probabilities for each band to be real such that $T_{0/\pi} = |t_{0/\pi}|^2 = \sqrt{1 - |r_{0/\pi}|^2}$. At this point, $S_K$ remains characterized by 16 free parameters. Choosing to parameterize the $U_i$ in terms of Euler angles:
Figure 3.5: The eight angular variables in the full formulation of the S-matrix, seven of which are linearly independent. $\theta_i$ corresponds to the processes which break small-momentum conservation and scatter electrons between the 0 and $\pi$ bands at lead $i$. $\phi_{ij} = \phi_i - \phi_j$ corresponds to the scattering phase acquired tunneling from lead $j$ to lead $i$ at valley $K$. While there are four independent $\theta_i$ angles, there are only three independent $\phi_{ij}$ as only the relative scattering phase matters, such that $\phi_{43} = \phi_{23} - \phi_{21} + \phi_{41}$. We have only displayed modes at $K$; an additional copy of this picture exists for modes at $K'$, related by time-reversal symmetry. This picture is valid for electrons with either spin, as our model system is SU(2) spin-invariant for all values of charge-sector interaction strengths.

\[
U_i = e^{i\phi_i \sigma^z} e^{i\theta_i \sigma^y} e^{i\alpha_i \sigma^z} e^{i\xi_i}. \tag{3.4.5}
\]

Recognizing that $\alpha_i$ and $\xi_i$ are just U(1)×U(1) transformations at each lead, we can gauge them out. We are then left with nine variables which have physical significance. The four $0 \leftrightarrow \pi$ mixing angles $\theta_i$ correspond to the breaking of small-momentum-conservation at lead $i$, the three independent linear combinations of scattering phases $\phi_{ij} = \phi_i - \phi_j$ each correspond to the phase acquired for electrons scattering from lead $j$ to lead $i$ at valley index $K$, and the two real tunneling
probabilities $T_0$ and $T_\pi$ characterize the extent to which the junction is pinched off for each band. These seven linearly independent angular variables (illustrated in Fig. 3.5) and two tunneling probabilities completely span the space of the gauge-independent, time-reversal-symmetric, spin- and valley-index-conserving problem with S-matrix,

$$S = S_K \oplus S_{K'} = S_K \oplus S_{K'}^T$$

which has rows and columns characterized by lead indexes $i, j$. This parameterization of the S-matrix in lead and band-index spaces is restated more explicitly in the beginning of Appendix 3.7.1.1.

In the subsequent sections, we will show how the surface where $\theta_i, \phi_{ij} = 0$ is not just a welcome simplification of the problem, but also the surface which contains all of the characteristic quantum critical points and their single relevant eigenvectors.

### 3.4.2 S-Matrix Renormalization under Weak Interactions

As discussed in 3.3.1, this system is characterized by two kinds of density-density interactions. Here, we relate the S-matrix to the single-particle Green’s function and then use diagrammatic perturbation theory in those two interactions to find the leading order corrections to the S-matrix and derive RG flow equations for our
system parameters [143, 199, 248]. We calculate the relevant physics on the high-symmetry surface where the interband scattering angles $\theta_i = 0$. In Appendix 3.7.1, we further calculate the RG flow for all nine S-matrix parameters, demonstrating that the angles $\theta_i, \phi_{ij}$ either flow back to this surface or are marginal and trivial at the quantum critical points.

3.4.2.1 Constructing the S-Matrix Renormalization Group

Scattering processes from one lead, band, and spin to another can be considered in terms of a single-electron thermal Green’s function

$$G_{ij}^{\alpha\beta, \sigma\sigma'}(x, \tau, x', \tau') = -i \left\langle T_{\tau} \left[ \psi_{i}^{a\alpha \sigma}(x, \tau) \psi_{j}^{b\beta \sigma'}(x', \tau') \right] \right\rangle $$  \hspace{1cm} (3.4.7)

where $T_{\tau}$ denotes imaginary time ordering and indexes $a, b = in, out$. In the absence of interactions

$$G_{ij}^{\alpha\beta, \sigma\sigma'}(z, z') = \frac{1}{2\pi i} \left( \begin{array}{cc} \delta_{ij} & (S_{ji})^* \\ \bar{S}_{ij}^{\alpha\beta} & \delta_{ij} \delta^{\alpha\beta} \end{array} \right) \delta_{\sigma\sigma'} $$  \hspace{1cm} (3.4.8)

where $z = \tau + ix$ and the rows and columns of $G_{ij}^{\alpha\beta}$ are the $in/out$ indexes such that elements proportional to $S_{ij}^{\alpha\beta}$ correspond to $in \leftrightarrow out$. Restricting ourselves to the interactions introduced in 3.3.1 (Eq. (3.3.2)), we can use diagrammatic pertur-
bation theory to calculate the leading order corrections to $G_{ij}^{\alpha\beta,\sigma\sigma'}$ in the presence of weak $u_+/-$, such that the Luttinger parameters $g_{+/-} = 1 + \epsilon_{+/-}$ and terms are kept up to $O(\epsilon_{+/-})$.

The one-loop corrections to the S-matrix are qualitatively similar to those in Ref. 199, with special care taken to properly sum at each vertex over the tensor structure of the interaction

$$\epsilon^{\alpha\beta\gamma\delta} = \epsilon_i \delta^{\alpha\beta} \delta^{\gamma\delta} + \epsilon_- \sigma_2^{\alpha\beta} \sigma_2^{\gamma\delta}$$

(3.4.9)

where $\alpha, \beta, \gamma, \delta$ are band indexes. Illustrated in Fig. 3.6, only two diagrams contribute to the renormalization of the single-particle Green’s function:

$$G^{\text{out in, } \alpha\beta, \sigma\sigma'}_{ij} = \frac{1}{2\pi i z - z'} \delta^{\sigma\sigma'}$$

(3.4.10)

with

$$S^{\alpha\beta}_{ij} = S_0^{\alpha\beta}_{ij} + 2 \times \frac{1}{4} \log \frac{\Lambda}{E} \sum_{A,B=0,1} \epsilon_A \epsilon_B \left[ \left( \sigma_A S_{ij} \sigma_B \right)^{\alpha\beta} \text{Tr} \left[ \sigma_A S_{ji}^{\dagger} \sigma_B \sigma_S S_{ji} \right] \right]$$

$$- \sum_{kl} \left( S_{ik} \sigma_A S_{lk}^{\dagger} \sigma_B S_{ij} \right)^{\alpha\beta} \text{Tr} \left[ \sigma_A S_{kl}^{\dagger} \sigma_B \sigma_S S_{kl} \right]$$

(3.4.11)
Figure 3.6: The two non-zero, non-canceling diagrams for $O(\epsilon^2)$ perturbation theory. Note that $i-l$ are spatial lead indexes and $\alpha - \delta, u-z$ are band indexes which are summed at each vertex over $\epsilon^{\alpha\beta\gamma\delta}$. $\sigma, \sigma'$ are spin indexes for which the $\delta^{\sigma\sigma'}$ within each Green's function has already been taken into account. Even though the system is spin invariant, the spin index on the loop, here $\sigma'$, must still be summed over its two values to calculate the physical RG flow. Each diagram contributes a logarithmic correction to the S-matrix which, when renormalized, leads to a term in Eq. (3.4.12).

where $\Lambda$ and $E$ are the ultraviolet and infrared cutoffs respectively. Traces refer to band index space, $\epsilon_{A/B} = \epsilon_{+/\mp}$, and $\sigma_{A/B} = 1, \sigma_z (\sigma_0, \sigma_1)$; tracing over the spin degree of freedom is implicit, which leads to the prefactor of 2. The two terms correspond to the diagrams (a) and (b) respectively in Fig. 3.6. We can derive flow equations for the elements of $S^\alpha\beta_{ij}$ by rescaling the cutoff $\Lambda \rightarrow \Lambda e^{-l}$,

$$
\frac{dS^{\alpha\beta}_{ij}}{dl} = \frac{1}{2} \sum_{A,B=0,1} \epsilon_A \epsilon_B \left[ (\sigma_A S_{ij} \sigma_B)^{\alpha\beta} \text{Tr}[\sigma_A S_{ji}^\dagger \sigma_B S_{ji}] \right]
$$

$$
- \sum_{kl} \left( S_{ik} \sigma_A S_{lk}^\dagger \sigma_B S_{lj} \right)^{\alpha\beta} \text{Tr}[\sigma_A S_{lk}^\dagger \sigma_B S_{lk}] . \tag{3.4.12}
$$

One can immediately observe that this implies that $\theta_i = 0$ is a fixed surface, since perturbative corrections to $S^{0\sigma}_{ij} = 0$ require multiplying by $S^{0\sigma}_{ij}$ in the above
equations. We can thus, for now, simplify our focus to the fixed surface where \( \theta_i = 0 \). In Appendix 3.7.1, we calculate the stability of the quantum critical points on this surface for a general set of \( \theta_i \) and \( \phi_{ij} \), and demonstrate that for physical values of \( g_- \) relative to \( g_+ \), the critical points are stable in all possible out-of-plane, \( \tau \)- and valley-symmetric directions.

Using our parameterization of \( S_{ij}^{\alpha\beta} \) on the \( \theta_i = 0 \) surface, we can exploit the matrix structure of the diagrammatic perturbations to obtain flow equations for the transmission probabilities for each band

\[
\begin{align*}
\frac{dT_0}{dl} &= -2T_0(1 - T_0) \left[ (\epsilon_+ + \epsilon_-)^2 (1 - 2T_0) + (\epsilon_+ - \epsilon_-)^2 (1 - 2T_\pi) \right] \\
\frac{dT_\pi}{dl} &= -2T_\pi(1 - T_\pi) \left[ (\epsilon_+ + \epsilon_-)^2 (1 - 2T_\pi) + (\epsilon_+ - \epsilon_-)^2 (1 - 2T_0) \right].
\end{align*}
\]

(3.4.13)

This system of equations obeys two key symmetries. First and foremost, like the QSH point contact described in Ref. 199, it is invariant under the pinch-off duality \( T_0/\pi \leftrightarrow (1 - T_0/\pi) \), which we introduced in 3.3.2. Eqs. (3.4.13) are also invariant under exchange of the band indexes 0 and \( \pi \). In the context of our renormalization group calculation, 0 and \( \pi \) are arbitrary labels for the band degree of freedom, and so even though this system contains stable fixed points with broken band-
Figure 3.7: RG flow of the variables $T_0/\pi$, which control the pinching off of the junction, calculated to quadratic order in the interactions $\epsilon_+/\epsilon_-$ (Eq. (3.4.13)), panels (a)-(c). Large circles correspond to stable fixed points and small circles indicate nontrivial quantum critical points. The flow is controlled by the ratio of the interaction strengths $\epsilon_-/\epsilon_+$. When $\epsilon_-/\epsilon_+ = 1$, the 0 and $\pi$ bands are completely decoupled and each one behaves individually as a copy of the QSH problem in Ref. 199 (a). For $\epsilon_-/\epsilon_+ > 0$, a set of intermediate fixed points exists which allows the 0 and $\pi$ bands to be pinched off independently (b). When $\epsilon_- = 0$, the quadratic theory predicts that a fixed line will exist $T_0 + T_\pi = 1$ (c). Higher-order corrections about this line, calculated in Appendix 3.7.2, infer flow along it back to the central quantum critical point $T_0 = T_\pi = 1/2$ (d).

index symmetry, the system of flow equations itself must be band-index symmetric. Graphically, these two symmetries manifest themselves as two mirror symmetries in Fig. 3.7: one about $T_0 + T_\pi = 1$ and the other about $T_0 = T_\pi$.

3.4.2.2 Fixed Points and Renormalization Group Flow

This system of flow equations can have as many as nine fixed points to quadratic order in the interactions (Fig. 3.7). The two corner fixed points at $T_0 = T_\pi = 0, 1$
are stable for all values of $\epsilon_-$. The central point at $T_0 = T_\pi = 1/2$ controls the transition between the CC and II corners and is related to the $T = 1/2$ critical point in the single-band TI QPC case [199]. As in that case, the existence of this central quantum critical point is mandated by the pinch-off duality $T_{0/\pi} \leftrightarrow 1 - T_{0/\pi}$.

The corner fixed points at $T_0 = 0$, $T_\pi = 1$ and $T_0 = 1$, $T_\pi = 0$ represent new, stable, single-electron-tunneling phases where only one of the bands is pinched off. We label these intermediate, mixed-band-character fixed points as “M Phases”. Transitions between the fully open or closed phases and these M phases are controlled by four fixed points which exist for $\epsilon_-/\epsilon_+ > 0$ (Figs. 3.7a, 3.7b). For $\epsilon_- = \epsilon_+$, the 0 and $\pi$ bands are completely decoupled and each one acts as a (spin-doubled) independent copy of the QSH problem in Ref. 199 (Fig. 3.7a). When $\epsilon_-/\epsilon_+ = 0$, Eq. (3.4.13) predicts that all of the intermediate transitions and stable fixed points will collapse onto a fixed line at $T_0 + T_\pi = 1$ (Fig. 3.7c). This $\epsilon_- = 0$ case represents a restoration of U(2) band-index symmetry locally at each lead under which the band indexes become trivial.

We can examine this fixed line in greater detail by expanding upon our bosonization calculations from 3.3.2. In Appendix 3.7.2, we increase the strength of $\pi \leftrightarrow \pi$ single-electron tunneling to drive from the CC phase towards an action about the M-phase corner fixed points for $g_- = 1$. Calculating higher-order correlation functions about this theory and expanding perturbatively again in the interactions, we discover additional fixed points:
\[ 1 - T_0 = T_\pi = \frac{48 \epsilon_-}{\pi^2 \epsilon_+^3}; \quad T_0 = 1 - T_\pi = \frac{48 \epsilon_-}{\pi^2 \epsilon_+^3} \quad (3.4.14) \]

where the second point is implied by the combination of mirror reflections about the pinch-off and band-index-exchange lines. Taking \( \epsilon_- \to 0 \), this theory exhibits flow back towards the central quantum critical point \( T_0 = T_\pi = 1/2 \) (Fig. 3.7d).

The simplest assumption would be to postulate that, to lowest order, this flow continues away from the vicinity of the M points without additional fixed points appearing. This implies that the fixed line at \( \epsilon_- = 0 \) is simply an artifact of the \( \mathcal{O}(\epsilon_+^2/\epsilon_-) \) perturbation theory and that for extremely small \( \epsilon_-/\epsilon_+ \), the M phase is unstable and flow lines in that region point towards the central quantum critical point \( T_0 = T_\pi = 1/2 \). From this information, we obtain Figure 3.8, a schematic which incorporates the quadratic-order RG flow and the higher-order corrections near the \( T_0 + T_\pi = 1 \) line. As highlighted by the red and purple arrows in that figure, each of the two classes of nontrivial quantum critical points is characterized by only a single relevant direction in the \( T_0 - T_\pi \) plane. All other out-of-plane \( \theta_i \) and \( \phi_{ij} \) directions are irrelevant or trivially marginal (Appendix 3.7.1).

### 3.4.2.3 Conductance Signatures and Universal Scaling Functions

For each class of quantum critical point, we can, knowing that its only relevant eigenvector lies on the \( \theta_i = 0 \) plane, use the quadratic-order flow equations to
calculate the universal conductance scaling and critical exponents to leading order in the interactions.

Returning to a discussion of reduced conductance matrixes from 3.3.2, we can express the left-to-right, two-terminal conductance $G_{XX}$ in terms of the S-matrix. The elements of the four-terminal conductance $G$ in the lead basis are related to the S-matrix by:

$$G_{ij} = \frac{2e^2}{h} \text{Tr}[\mathbb{1} - S_{ij}^\dagger S_{ij}]$$  \hspace{1cm} (3.4.15)

where $i, j$ are lead indexes $1 - 4$ such that the matrix

$$G = \frac{2e^2}{h} \begin{pmatrix}
2 & -T_+ & 0 & -(2 - T_+) \\
-T_+ & 2 & -(2 - T_+) & 0 \\
0 & -(2 - T_+) & 2 & -T_+ \\
-(2 - T_+) & 0 & -T_+ & 2
\end{pmatrix}$$  \hspace{1cm} (3.4.16)

where $T_\pm = T_0 \pm T_\pi$ and the factor of 2 on the conductance is due to electron spin degeneracy. The linear combinations of lead currents $I_{1-4}$ which give $I_{X,Y,Z}$ are a result of, in combination with the requirement $\sum_i I_i = 0$, 

103
Figure 3.8: A schematic phase diagram, in terms of left-to-right conductance, within the $T_0 - T_\pi$ plane, combining information from Eq. (3.4.13) and Appendix 3.7.2. There are two classes of quantum critical points. The central point controls transitions between the fully open (CC) phase and the fully pinched-off (II) phase. Four additional critical points on the edges control transitions between the CC/II phases and an intermediate mixed (M) phase in which the two bands have differing conductance contributions. The width of the M phase is $\mathcal{O}(\epsilon_-/\epsilon_+)$. 

\[
\begin{pmatrix}
I_X \\
I_Y \\
I_Z
\end{pmatrix}
= 
M^T
\begin{pmatrix}
I_1 \\
I_2 \\
I_3 \\
I_4
\end{pmatrix}
\tag{3.4.17}
\]

where 

\[
M = \frac{1}{2}
\begin{pmatrix}
1 & 1 & 1 \\
-1 & 1 & -1 \\
-1 & -1 & 1 \\
1 & -1 & -1
\end{pmatrix}
\tag{3.4.18}
\]
such that

\[
G^{XYZ} = M^T G M = \frac{4e^2}{h} \begin{pmatrix}
T_+ & 0 & 0 \\
0 & 2 - T_+ & 0 \\
0 & 0 & 2
\end{pmatrix}.
\] (3.4.19)

This confirms the result from 3.3.2 that, for the valley-conserving problem, \(G_{ZZ}\) is quantized to be \(8e^2/h\) regardless of the junction state. This reduction also confirms that, in terms of the S-matrix elements,

\[
G_{XX} = \frac{4e^2}{h} (T_0 + T_\pi) = \frac{8e^2}{h} - G_{YY}.
\] (3.4.20)

With the structure of the conductance matrix established we can analyze the finite-temperature conductance transitions near each transition voltage \(V^*_G\).

First, we will consider the direct I-I phase transition, for which \(G_{XX}\) scales from 0 to \(8e^2/h\). We can write the conductance in its scaling form

\[
G_{XX,A}(\Delta V_G, T) = 8\frac{e^2}{h} G_A \left( c \frac{\Delta V_G}{T^\alpha_A} \right),
\] (3.4.21)

where \(\Delta V_G = V_G - V^*_{G,A}\) in Fig. 3.9, \(c\) is a non-universal constant, and the subscript \(A\) on \(G\) and \(\alpha\) denotes the direct quantum phase transition between the
II and CC phases. Observing that infinitesimal movement of $T_-$ away from 0 is irrelevant (Fig. 3.8), we can set $T_- = 0$ and characterize the conductance transition from II-CC with a single parameter,

$$\frac{dT_+}{dl} = -2(\epsilon_+^2 + \epsilon_+^2)T_+(2 - T_+)(1 - T_+). \quad (3.4.22)$$

This equation can be integrated to determine the crossover scaling function. Taking $T_+ = T_+^0$ at $l = 0$,

$$\frac{T_+^0(2 - T_+^0)}{(1 - T_+^0)^2} e^{-4(\epsilon_+^2 + \epsilon_+^2)t} = \frac{T_+(2 - T_+)}{(1 - T_+)^2} \quad (3.4.23)$$

where we have purposefully left $T_+(l)$ in its implicit form to provide a framework for the more mathematically complicated II-M transition analysis later in this section. As one adjusts the gate voltage, $T_+^0$ passes through 1 at $V_G = V_{G,A}^*$, such that near the transition $\Delta V_G \propto T_+^0 - 1$. To determine the critical behavior, we can therefore expand $T_+^0$ around this value. Finite temperature $T$ can be taken into consideration by cutting off the renormalization group flow $l$ at $\Lambda e^{-l} \propto T$. Taking $\Delta V_G, T \to 0$ at an arbitrary ratio, the previous equation can be rewritten

$$\frac{1}{(2X)^2} \frac{G_A(1 - G_A)}{(1 - 2G_A)^2} \quad (3.4.24)$$
Figure 3.9: A reproduction of Figure 3.8 with dashed lines overlaid to indicate possible voltage curves. As the gate voltage $V_G$ winds along a voltage curve, whose exact curvature is dictated by experimental specifics, it passes directly from the II to the CC region along a curve like (a) or indirectly, passing along the way through an intermediate M phase along a curve like (b). At zero temperature, the left-to-right conductance $G_{XX}$ will therefore undergo a direct transition from $0 \to 8e^2/h$ along (a) or one with an intermediate step up to $4e^2/h$ along (b). This behavior motivates us to search for the finite-temperature scaling of these conductance transitions for $V_G \sim V_{G,A}^*$ (a), or for $V_G \sim V_{G,B}^*$ and $V_G \sim V_{G,C}^*$ (b).

or explicitly inverted

$$G_A(X) = \frac{1}{2} \left[ 1 + \frac{X}{\sqrt{1 + X^2}} \right]$$

(3.4.25)

where $T_+ = 2G_A$ such that $X \propto \Delta V_G / T^{2(\epsilon_+^2 + \epsilon_-^2)}$.

$$\alpha_A = 2(\epsilon_+^2 + \epsilon_-^2)$$

(3.4.26)

is the universal critical exponent for the II-CC quantum phase transition. Fig-
Figure 3.10 shows $G_A$ at finite temperatures, noting that it collapses onto a step function at $T/c^{1/\alpha} = 0$ and that it has a crossover point pinned at $G_A = 1/2$ for all values of interaction, making it identical to the T-R scaling function for weak interactions in the related Quantum Spin Hall problem [199]. When $\epsilon_- = 0$ and the only transitions are directly from II-CC, $\alpha_A = 4\alpha_{QSH}$, where $\alpha_{QSH}$ is the T-R critical exponent in Ref. 199. This factor of 4 accounts for the fact that even though here only a single linear combination of indexes is being pinched off, the diagrams which contribute to the flow equations still live in a matrix space which is four times as large as that of the comparable Quantum Spin Hall problem.

Obtaining the critical exponent and scaling function for the II-M quantum phase transition is procedurally identical. As an example, we will choose the bottom right transition point in Fig. 3.9 for our calculation, though that point is restricted to be the same as the one characterizing the finite $T_\pi$ II-M transition by band-index-exchange symmetry. The quantum critical point is located at $T_\pi = 0, T_0 = \gamma/2$ where

$$\gamma = 1 + \frac{(\epsilon_- - \epsilon_+)^2}{(\epsilon_- + \epsilon_+)^2}.$$  \hspace{1cm} (3.4.27)

First and foremost, we can note that when $\gamma = 2, \epsilon_- = 0$ and there is no more available phase space (at quadratic order) for the II-M transition to exist. Near this case, the M phase will exist in a vanishing area of phase space and most
Figure 3.10: The two classes of universal scaling functions as functions of external gate voltage: $G_A$ describes the direct II-CC quantum phase transition and $G_B$ describes the II-M transition, plotted in panels (a) and (b) respectively. Here, we have plotted $\epsilon_+ = 0.212$, $\epsilon_- = 0.071$, such that $\gamma = 1.25$. The curves are plotted for increasing temperature, with the red, orange, green, and blue curves representing $T/\epsilon^{1/\alpha} = 0$, $10^{-5}$, $10^{-2.5}$, and $1 V^{1/\alpha}$ respectively in equations (3.4.24) and (3.4.31). Note that the crossover value of $G_A$ is fixed to be $1/2$, whereas the crossover value for $G_B$ is instead at $\gamma/2$, where $\gamma$ varies from 1 to 2 continuously as a function of interaction strength.

transitions will be controlled by the central quantum critical point in Figure 3.8. However, in Appendix 3.7.1 we have only analytically calculated the stability of the II-M quantum critical point to linear order in $\epsilon_-$, whereas our analysis of the critical behavior of the II-M transition is up to $O(\epsilon^2)$. We believe it reasonable to assume that this stability extends up to quadratic order in the interactions such that these quantum critical points still describe the relevant physical transitions in this problem.

For the II-M transition, the conductance jumps from $G_{XX} = 0 \to 4\epsilon^2/h$, with here the $T_0$ axis being the only relevant direction. For this transition then, $G_{XX} = \frac{4\epsilon^2}{h}T_0$. Expressing the conductance in its scaling form

109
where again $\Delta V_G$ is the external gate voltage, $c$ is a non-universal constant that may certainly differ from the $c$ in the II-CC transition, and the subscript $B$ denotes that transition between the II-M phases. Taking $T_\pi = 0$, the conductance transition from II-M is characterized by the flow of a single parameter,

$$
\frac{dT_0}{dl} = -2\gamma(\epsilon_+ + \epsilon_-)^2 T_0 (1 - T_0) \left(1 - \frac{2T_0}{\gamma}\right).
$$

(3.4.29)

We can determine the crossover scaling function by integrating this equation. Taking $T_0 = T_0^0$ at $l = 0$,

$$
\frac{T_0^0(1 - T_0^0)^{\frac{1}{\frac{3}{2} - 1}}}{\left(1 - \frac{2T_0^0}{\gamma}\right)^{\frac{2}{\gamma} \left(\frac{1}{\frac{3}{2} - 1}\right)}} e^{-2\gamma(\epsilon_+ + \epsilon_-)^2 l} = \frac{T_0(1 - T_0)^{\frac{1}{\frac{3}{2} - 1}}}{\left(1 - \frac{2T_0}{\gamma}\right)^{\frac{2}{\gamma} \left(\frac{1}{\frac{3}{2} - 1}\right)}}.
$$

(3.4.30)

As before, we can cut off the renormalization group flow at finite temperature $T \propto \Lambda e^{-l}$ and note that the gate voltage $V_G = V_{G,B}^*$ when $T_0^0$ passes through $\gamma/2$, such that near the transition $\Delta V_G \propto T_0^0 - \gamma/2$. Again taking $\Delta V_G, T \to 0$ at an arbitrary ratio, we can finally arrive at an implicit equation for $G_B(X)$,
Figure 3.11: The universal scaling function $G_B$ which characterizes the II-M phase transition, plotted for $T/c^{3/\alpha} = 10^{-3}$ $V^{1/\alpha}$ and $g_+ = 1.212$. The blue, green, orange, and red curves are plotted at $g_- = 1.019$, 1.047, 1.071, and 1.212 respectively. The critical value of $G_B$ for which the conductance flow changes from the II phase to the M phase occurs at the intersection of each curve with the $\Delta V_G = 0$ line, and varies as a function of the ratio of the interaction strengths $g_-/g_+$. When $g_- = g_+$, $G_B$ takes on the same functional form as $G_A$ in Fig. 3.10, though with a different critical exponent $\alpha_B \neq \alpha_A$. At $T = 0$ K, all of these curves collapse onto the same step function; they are increasingly distinguishable as temperature is increased.
\[
\frac{1}{(\frac{2X}{\gamma})^2} = \frac{G_B^{(2-\gamma)}(1 - G_B)^{\gamma}}{(1 - 2G_B/\gamma)^2}
\]

(3.4.31)

where \( T_0 = G_B \) such that \( X \propto \Delta V_G/T^{(\epsilon_+ + \epsilon_-)2(2-\gamma)} \). We can note that this equation reduces to Eq. (3.4.24) for \( \gamma = 1 \). That case represents \( \epsilon_- \to \epsilon_+ \), for which \( T_0 \) and \( T_\pi \) act as independent copies of the Quantum Spin Hall problem in Ref. 199, but in a higher-dimensional space. Therefore,

\[
\alpha_B = (\epsilon_+ + \epsilon_-)^2 \gamma (2 - \gamma) = \alpha_A (2 - \gamma)
\]

(3.4.32)

is the universal critical exponent for the II-M transition. Confirming the relationship to the QSH point contact problem, setting \( \gamma = 1 \) gives \( \alpha_B|_{\epsilon_-=\epsilon_+} = 2\alpha_A|_{\epsilon_-=0} = 8\alpha_{QSH} \). Figure 3.10 shows \( G_B \) as a function of \( \Delta V_G \) at different temperatures, noting that at zero temperature it is also a step function, indistinguishable from \( G_A \), but that at finite temperature it is defined by a crossover value of \( \gamma/2 \) which in general differs from that of \( G_A \) (Fig. 3.11).

Taking advantage of the duality between the II and CC phases, we can relate the remaining conductance crossover function, one which characterizes the M-CC phase transition, to \( G_B \). We can write the conductance in its scaling form
where \( c \) is yet another non-universal constant and \( C \) denotes that M-CC transition. By pinch-off symmetry, we know that \( G_{YY} \) for the CC\( \rightarrow \)M transition has to be equivalent to \( G_{XX} \) for the II\( \rightarrow \)M transition, therefore for the M\( \rightarrow \)CC transition,

\[
G_{XX,C} = \frac{4e^2}{\hbar} + \frac{4e^2}{\hbar} G_C \left( c \frac{\Delta V_G}{T^{\alpha_C}} \right) \tag{3.4.33}
\]

\[
G_{YY,C} = 4e^2 h + 4e^2 h G_C \left( -c \frac{\Delta V_G}{T^{\alpha_C}} \right) \tag{3.4.34}
\]

and utilizing Eq. (3.4.20),

\[
G_{XX,C} = \frac{8e^2}{\hbar} G_B \left( -X \right) \tag{3.4.35}
\]

such that we finally deduce

\[
G_C(X) = 1 - G_B(-X) \tag{3.4.36}
\]

where \( X \propto \Delta V_G/T^{\alpha_C} \) and

\[
\alpha_C = \alpha_B \tag{3.4.37}
\]
for weak interactions.

3.5 Discussion

In this chapter, we have computed the conductance signatures of the four-terminal intersection of two bilayer graphene domain walls. These domain walls can be induced by the presence of a perpendicular electric field and a change in either electric field direction or interlayer stacking. When valley-index is conserved, the domain walls are Luttinger liquids described with two non-trivial interaction parameters $g_{\pm}$. The junction is analogous to a point contact and can be analyzed naturally using the language of quantum point contacts. As with a Quantum Spin Hall point contact, the physics of the junction is best understood in terms of reduced, two-terminal conductances. When interactions are strongly attractive ($g_{\pm} < 1/4$) or strongly repulsive ($g_{\pm} > 4$), the left-to-right conductance can be strictly dominated by nonzero charge and valley conductances respectively. For weaker interactions ($g_{\pm} \approx 1$), both left-to-right conductances are nonzero and there exist several stable phases characterized by single-electron tunneling. Transitions between these phases are governed at low temperatures by universal scaling functions and critical exponents, which differ from those in the single-band QSH case and are functions of the two Luttinger parameters.

We now briefly discuss the task of experimentally measuring the physics in this
chapter. First and foremost, the existence of a single domain wall in bilayer graphene requires prohibiting scattering between valleys $K$ and $K'$. Valley-index-breaking perturbations are strongly relevant and will significantly change the physics in both isolated domain walls and for the junction structures at their intersections. To this end, short-range disorder must be kept smooth on the scale of the lattice. Recent experiments have shown promising results in this direction, with fabricated samples showing single domain wall conductances up to nearly the quantized clean limit of $4e^2/h$ [101]. Beyond these results, one should then attempt to verify the Luttinger liquid physics at a single domain wall by measuring the tunneling conductance at several low temperatures and its collapse onto a universal scaling function with critical exponent $\alpha_T$. In junction structures, the conservation of valley index can be confirmed by measuring the quantization of the reduced conductance element $G_{zz}$.

Creating a multi-terminal junction like the ones we describe poses several fabrication and analysis difficulties which must be overcome to measure the point-contact physics in this chapter. Forming a four-terminal junction of electric-field-induced domain walls requires patterning leads on the top and bottom of each of the four bulk regions, as well as a gate on the junction to control the weak-interaction pinch-off transition. Forming a junction from layer-stacking domain walls requires patterning fewer leads, but as clearly demonstrated in the samples in Ref. 5, the three-fold symmetry of the underlying graphene lattice restricts intersections of these domain walls to be six-terminal structures. Conductance transitions in these six-terminal structures can be calculated and analyzed using the framework estab-
lished in this chapter, though the task will be algebraically more intensive.

Tuning the two Luttinger parameters $g_\pm$ can be accomplished through turning a combination of experimental knobs. The strength of the overall effective Coulomb interaction can be altered for the domain wall states by tuning their widths with the strength of the perpendicular electric field. These changes will be mainly reflected in $g_+$, as it contains long-range contributions from the overall Coulomb interaction. The other Luttinger parameter, however, can only be adjusted by tuning short-range interactions. This can be accomplished by testing samples on a variety of substrates. Working in order of increasing dielectric strength, one can work through a suspended sample, a silicon dioxide substrate, or a boron nitride substrate to tune down $g_-$. Several simplifications and assumptions in this chapter may not be exactly present under experimental conditions. The assumption that all domain walls in the sample have the same values of the Luttinger parameters requires that the perpendicular electric field strength be globally uniform in magnitude in the bulk regions and change in direction similarly smoothly across electric-field-induced domain walls. It also requires that there are no strong local variations in the dielectric strength and coupling of the underlying substrate. The physics of junctions may be significantly altered if these conditions are not realized experimentally; we have not investigated point contacts at the intersections of two domain walls with differing interaction strengths. We also only calculated universal scaling functions
to leading order in the interactions about the noninteracting point $g_+ = g_- = 1$. When interactions become stronger and single-electron tunneling is no longer the least irrelevant operator, the critical exponents $\alpha_{A/B}$ in the left-to-right conductance transitions may change significantly in their dependences on the interaction strengths, as they do in Ref. 199. Finally, we assumed that the Fermi energy was exactly at the particle-hole-symmetric point such that $v_{F,0} = v_{F,\pi} = v_F$. In practice, it will be quite difficult to exactly tune the Fermi energy to this point, and so for most experimental realizations, $0 \leftrightarrow \pi$ exchange symmetry in the variables will be broken. For our analysis, the effects of this can be realized by replacing the equal band-index-exchange symmetry which we exploited with one which flips band index and rescales variables by $v_{F,0}/v_{F,\pi}$. This will result in changes to the scaling dimension calculations in Section 3.3.2 and a relaxation of mirror symmetry about $T_0 = T_\pi$ in Figure 3.8.

### 3.6 Chapter Acknowledgments

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3.7 Appendix

3.7.1 Stability of Quantum Critical Points on the $\theta_i = 0$ Surface

In this appendix, we confirm analytically the stability of the two classes of quantum critical points in Fig. 3.8 which control the transitions between single-electron-tunneling phases. Here, we begin with the general flow equation for elements of the S-matrix (Eq. (3.4.12)), leaving free the $\theta_i$ and $\phi_{ij}$ variables in the full S-matrix formulation from 3.4.1. As the complexity of this calculation greatly grows with each power of $\epsilon_-$ taken into consideration, we will only here carry out our stability analysis to quadratic order in $\epsilon_+$ and linear order in $\epsilon_-$. Our methodology can be used to analytically calculate higher-order terms, but we believe it reasonable to truncate the calculation at this order and that the stability should carry over to the $\mathcal{O}(\epsilon_+^2)$ calculation used to produce the phase diagrams and scaling functions in 3.4.2. Additionally, numerical estimates find $g_- < g_+$ for a large range of system parameters [110], therefore the limitation to terms of order $\mathcal{O}(\epsilon_+\epsilon_-, \epsilon_-^2)$ is physically motivated.

We can exploit the matrix structure of the diagrammatics by taking several traces of S-matrix products. Derivatives of these traces exploit the matrix structure of the flow equation, effectively closing the external legs of the diagrams in Fig. 3.6 into additional loops. We will follow through this calculation completely for a single trace ($\text{Tr}[S_{ij}^\dagger \sigma_z S_{ij}]$) and then show how taking linear combinations of these traces
results in a flow equation for $\theta_1$. All remaining $d\theta_i/dl$ can be obtained by exploiting cyclic reindexing and pinch-off symmetries.

3.7.1.1 Flow Equations for $\theta_i$ Band Mixing Angles and $\phi_{ij}$ Scattering Phases

To begin this process, let us rewrite S-matrix elements in the $2 \times 2$ band space using a simplified version of Eqs. (3.4.3), (3.4.5):

$$S_{ij}^{\alpha\beta} = (U_i^\dagger D_{ij} U_j)^{\alpha\beta}$$

$$U_i = e^{i\theta_i}$$

$$D_{ij} = a_{ij} 1 + b_{ij} \sigma_z$$

$$a_{ij} = \frac{1}{2} (d_{ij}^0 + d_{ij}^\pi)$$

$$b_{ij} = \frac{1}{2} (d_{ij}^0 - d_{ij}^\pi)$$

(3.7.1)

$$d^a = \begin{pmatrix}
0 & t^a e^{i\phi_A} & 0 & r^a e^{i\phi_B} \\
-t^a e^{i\phi_A} & 0 & -r^a e^{i\phi_C} & 0 \\
0 & -r^a e^{i\phi_C} & 0 & t^a e^{i\phi_D} \\
-r^a e^{i\phi_C} & 0 & t^a e^{i\phi_D} & 0 \\
\end{pmatrix}$$

(3.7.2)

where $d^a_{ij}$ is a collection of scalars in the band index space with $a = 0, \pi$, 119
\( \phi_{ij}^0 = -\phi_{ij}^\pi = \phi_{ij} \) and all matrix operations only involve the \( \alpha, \beta = 0, \pi \) indexes.

Transmission probabilities are normalized for each band such that \((t^a)^2 + (r^a)^2 = 1\)
and the labeling \( A - C \) on the phases corresponds to:

\[
\begin{align*}
\phi_A &= \phi_{21} = \phi_2 - \phi_1 \\
\phi_B &= \phi_{41} \\
\phi_C &= \phi_{23} \\
\phi_D &= \phi_{43} = \phi_B - \phi_A + \phi_C. 
\end{align*}
\]

We’ll begin by calculating three traces:

\[
\begin{align*}
\text{Tr}[S_{ij}^\dagger S_{ij}] &= |d_{ij}^0|^2 + |d_{ij}^\pi|^2 \\
\text{Tr}[S_{ij}^\dagger \sigma_z S_{ij}] &= (|d_{ij}^0|^2 - |d_{ij}^\pi|^2) \cos \theta_i \\
\text{Tr}[S_{ij}^\dagger \sigma_x S_{ij}] &= (|d_{ij}^0|^2 - |d_{ij}^\pi|^2) \sin \theta_i. 
\end{align*}
\]

We can then differentiate and take weighted linear combinations of these traces
to obtain explicit flow equations for \( \theta_i \). Specializing to \( i, j = 1, 2 \),
\begin{equation}
(T_0 - T_\pi) \frac{d\theta_1}{dl} = (\cos \theta_1) \frac{d}{dl} \text{Tr}[S_{12}^\dagger \sigma_x S_{12}] - (\sin \theta_1) \frac{d}{dl} \text{Tr}[S_{12}^\dagger \sigma_z S_{12}] \tag{3.7.5}
\end{equation}

where \( T_{0/\pi} = |t^{0/\pi}|^2 \). Now, we can examine, in detail, the process of using the diagrammatics (Eq. (3.4.12)) to calculate one of these derivatives, namely \( \frac{d}{dl} \text{Tr}[S_{12}^\dagger \sigma_z S_{12}] \). All other trace derivatives, while varying in signs and specifics, follow procedurally from this example.

First, by using the cyclic index definition of the trace, we can see that the derivative of the trace is equal to the trace of the chain rule derivative:

\begin{equation}
\frac{d}{dl} \text{Tr}[S_{12}^\dagger \sigma_z S_{12}] = \text{Tr}\left[ \frac{dS_{12}^\dagger}{dl} \sigma_z S_{12} \right] + \text{Tr}\left[ S_{12}^\dagger \sigma_z \frac{dS_{12}}{dl} \right] = \text{Tr}\left[ S_{12}^\dagger \sigma_z \frac{dS_{12}}{dl} \right] + C.C. \tag{3.7.6}
\end{equation}

where for the second equality we exploited the cyclic nature of the trace to reduce this step to the calculation of one, albeit large, trace. In this case, the trace of the derivative is real, but in the next section where we calculate \( d\phi_{ij}/dl \), it will not be and the addition of the complex conjugate cannot be overlooked.
From here, the calculation amounts to taking the traces of terms which contain products of two or four S-matrices. While the products of two, in the form of Eq. (3.7.4), can be calculated by rote algebra without much difficulty, the terms with four S-matrices require a bit more manipulation.

We calculate the traces of products of four S-matrices by both recognizing a pattern in the assignment of signs to the products of $a_{ij}, b_{ij}$ and with a careful treatment of commutivity issues. Consider first the simplest example, $\text{Tr}[S_{l2}^{\dagger}S_{lk}S_{1k}^{\dagger}S_{12}]$. Without any additional Pauli matrices, the $U_i$ rotations all cancel out pairwise, resulting in:

\[
\text{Tr}[S_{l2}^{\dagger}S_{lk}S_{1k}^{\dagger}S_{12}] = \text{Tr}[(a_{l2}^{\ast} \mathbb{1} + b_{l2}^{\ast} \sigma_z)(a_{lk} \mathbb{1} + b_{lk} \sigma_z) \newline (a_{1k}^{\ast} \mathbb{1} + b_{1k}^{\ast} \sigma_z)(a_{12} \mathbb{1} + b_{12} \sigma_z)]. \tag{3.7.7}
\]

One might be concerned that converting this to a useful form, one with $d_{ij}^{0/\pi}$ where S-matrix elements can just be read off, would be a daunting and terrible task. However, converting to $d_{ij}^{0/\pi}$ basis is equivalent to summing over all of the ways to choose $+$ and $-$ signs for the cross terms, and so for every single one of these four S-matrix traces, all of the cross terms cancel. Our trace is reduced to the quite simple form:
\[
\text{Tr}[S^\dagger_{12} S_{1k}^\dagger S_{12}^\dagger] = \sum_{a=0,\pi} (d^a_{12})^* d^a_{ik} (d^a_{1k})^* d^a_{12}.
\] (3.7.8)

Worth noting is that this picture is significantly complicated by the addition of Pauli matrices between S-matrix factors, due to the fact that \([U_i, \sigma_{z/x}] \neq 0\). While the complexity doesn’t significantly increase for the addition of a single Pauli matrix, as it can be absorbed into the definition of \(D_{ij}\), it does for two or more Pauli matrices. This can be seen at the level of the two-S-matrix trace, where commutivity issues lead to the addition of a second term:

\[
\text{Tr}[\sigma_z S^\dagger_{ij} \sigma_z S_{ij}] = \cos \theta_i \cos \theta_j \left[ |d^0_{ij}|^2 + |d^\pi_{ij}|^2 \right]
+ \sin \theta_i \sin \theta_j \left[ d^0_{ij} (d^\pi_{ij})^* + (d^0_{ij})^* d^\pi_{ij} \right].
\] (3.7.9)

For the four-S-matrix traces, the weighting of the cross terms is altered by the anticommutativity of the Pauli matrices and while only two terms remain for each trigonometric function of \(\theta_i\), they are different than the simple form of Eq. (3.7.8) and contain possible terms which mix 0 and \(\pi\).

As the number of Pauli matrices inserted into these traces increases linearly with the power of \(\epsilon_-\) to which we expand, we have chosen for the sake of simplicity and
clarity to expand only to linear order in $\epsilon_-$. Though our analysis in section 3.4.2.2 continues to $\mathcal{O}(\epsilon_-^2)$, we believe that the stability deduced here should carry over to higher order terms.

With our calculation machinery established, we can produce a flow equation for the $0 \leftrightarrow \pi$ mixing at lead 1:

$$\frac{d\theta_1}{dl} = -\epsilon_+ \epsilon_- \left\{ \sin 2\theta_1 [T_0 (1 - T_\pi) + T_\pi (1 - T_0)] + \sin 2\theta_2 \cos (2\phi_{21}) \sqrt{T_0 T_\pi [2 - T_0 - T_\pi]} ight. \\
+ \left. 2 \sin 2\theta_3 \cos (2\phi_{31}) \sqrt{T_0 (1 - T_0) T_\pi (1 - T_\pi)} + \sin 2\theta_4 \cos (2\phi_{41}) \sqrt{(1 - T_0)(1 - T_\pi)[T_0 + T_\pi]} \right\},$$

(3.7.10)

Flow equations for the remaining three mixing angles can be generated by exploiting underlying symmetries of the problem. The set of nine independent variables which characterizes the S-matrix obeys three symmetries. Two “pinch-off” symmetries exist; the duality between the fully closed (II) and fully open (CC) single-electron phases implies that the system of flow equations is invariant with respect to the exchange $T_{0/\pi} \leftrightarrow (1 - T_{0/\pi})$ and either the exchange of lead indexes 2 $\leftrightarrow$ 4 or 1 $\leftrightarrow$ 3. The third symmetry is a cyclic relabeling of the lead indexes as well as an exchange of the definitions of pinched off and open, due to the
system’s invariance under properly-treated (with respect to valley) 90° rotations. Therefore the system is also invariant under the exchange $T_{0/\pi} \leftrightarrow (1 - T_{0/\pi})$ and $1 \rightarrow 2$, $2 \rightarrow 3$, $3 \rightarrow 4$, and $4 \rightarrow 1$. Independent calculations of $d\theta_i/dl$ confirm these properties.

We can see immediately that for $\epsilon_- = 0$, all $\theta_i$ are marginal. In this case, the system has U(2) symmetry at each lead and all band index rotations can be gauged out. The dependence of $d\theta_i/dl$ on $\theta_{j \neq i}$ can also be suppressed by tuning the scattering phase $\phi_{ij}$ closer to $\pi/4$, which amounts to having a $\pi/2$ scattering phase difference between the 0 and $\pi$ bands.

Calculating the flow equations for scattering phases $\phi_{ij}$ requires, conversely, tracing over open paths in diagrams, which allows phase to accumulate throughout the summation instead of being canceled out pairwise as frequently occurred in the calculation of $d\theta_i/dl$. Specializing for the moment towards obtaining $d\phi_A/dl$, we can note the following:

\begin{align*}
\text{Tr}[S_{12}] &= (t_0 e^{i\phi_A} + t_\pi e^{-i\phi_A}) \cos \left(\frac{\theta_1 - \theta_2}{2}\right) \\
|\text{Tr}[S_{12}]|^2 &= \cos^2 \left(\frac{\theta_1 - \theta_2}{2}\right) \left[T_0 + T_\pi + 2\sqrt{T_0 T_\pi} \cos 2\phi_A\right] \\
(3.7.11)
\end{align*}
where the correspondence between the subscripts $A-D$ and the lead indexes $i, j$
comes from Eq. (3.7.3). This can be differentiated, and, with a considerable amount
of algebra, used to obtain first order flow equations for the scattering phases. While
the specifics of this calculation differ from those of obtaining the $d\theta_i/dl$, the key
point about the summation over $+$ and $-$ possibilities when converting to the $d_{ij}^{\theta/\pi}$
basis remains for both the one- and three-S-matrix products here, again greatly
simplifying the algebra for the required trace calculations. Utilizing this fact, we
obtained an explicit flow equation for scattering phase $\phi_A$:

$$
d\phi_A/dl = \frac{1}{2} \epsilon_+ \epsilon_- \tan \left( \frac{\theta_1 - \theta_2}{2} \right) \left\{ (\sin 2\theta_1 - \sin 2\theta_2) \sin (2\phi_A) \sqrt{T_0 T_{\pi}} (2 - T_0 - T_{\pi}) 
+ \sin 2\theta_3 \sqrt{(1 - T_0)(1 - T_{\pi})} \left[ (T_0 + T_{\pi}) \sin (2\phi_C) - 2 \sqrt{T_0 T_{\pi}} \sin (2(\phi_A - \phi_C)) \right] 
- \sin 2\theta_4 \sqrt{(1 - T_0)(1 - T_{\pi})} \left[ (T_0 + T_{\pi}) \sin (2\phi_B) - 2 \sqrt{T_0 T_{\pi}} \sin (2(\phi_A - \phi_B)) \right] \right\}.
$$

(3.7.12)

The flow equations for $\phi_{B-D}$ can be obtained by exploiting pinch-off and cyclic
symmetries as well as the redundancy of $\phi_D$ (Eq. (3.7.3)). As with the $\theta_i$, one can
observe that for the $U(2)$ symmetric case of $\epsilon_- = 0$, all $\phi_{ij}$ are also marginal and can
be gauged away. One can also observe that $d\phi_{ij}/dl = 0$ when $\theta_i = \theta_j$, as in that case
there is no relative interband scattering between leads $i$ and $j$ and $\phi_{ij}$ can be gauged
out. Only two unique stability calculations are required, as the four critical points
on the boundary of the square are related by pinch-off and band-index-exchange symmetries.

### 3.7.1.2 Quantum Critical Point Stability

We can now utilize the flow equations for $\theta_i$ and, to a lesser extent, $\phi_{ij}$ to determine the stability of the $\theta_i = \phi_{ij} = 0$ surface quantum critical points in Fig. 3.8.

We will begin by considering the $T_0 = T_\pi = 1/2$ central quantum critical point, which controls the direct transition between the fully pinched-off (II) and fully-open (CC) phases. Expanding the $\theta_i$ to linear order:

$$\begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix} = \begin{bmatrix} -\epsilon_- & -\epsilon_- & M \\ -\epsilon_- & -\epsilon_- & M \\ M & M & M \\ M & M & M \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix}$$

(3.7.13)

$$M_{ij} = \cos 2\phi_{ij}$$

(3.7.14)

which gives two Lyapunov exponents of zero and two of $\lambda_\pm = -2\epsilon_+\epsilon_- \left\{ 1 \pm \frac{1}{4} \sqrt{\sum_{i,j} \cos 4\phi_{ij}} \right\}$. Both $\lambda_\pm$ eigenvalues are either zero or negative for all choices of the independent $\phi_{A-C}$. Given the high symmetry of this central quantum critical point, it is unlikely
that the $\lambda = 0$ marginal directions correspond to instabilities at higher orders.

The four external critical points which control the transitions to and from the mixed (M) phase can be handled similarly, but with an attention to the expansions used to arrive at this analysis. As our model is invariant under global exchange $0 \leftrightarrow \pi$ and the pinch-off symmetries, we perform stability analysis on just one of the four critical points and relate the rest by symmetry.

Choosing the critical point at $T_0 = 0, T_\pi = \gamma/2$, we can again construct a stability matrix:

$$
\frac{d}{dl} \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{pmatrix} = -\epsilon_+ \epsilon_- \gamma N \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{pmatrix}
$$

(3.7.15)

$$
N = 1 + \sqrt{1 - \frac{\gamma}{2}} \begin{pmatrix} 0 & 0 & 0 & \cos 2\phi_B \\ 0 & 0 & \cos 2\phi_C & 0 \\ 0 & \cos 2\phi_C & 0 \\ \cos 2\phi_B & 0 & 0 \end{pmatrix}
$$

(3.7.16)

Acknowledging that, as we have expanded to linear order in $\epsilon_-, \gamma \approx 2 - 4\epsilon_-/\epsilon_+$, all of the off-diagonal terms become infinitesimal and we are left with:
\[
\frac{d}{dl} \begin{pmatrix}
\theta_1 \\
\theta_2 \\
\theta_3 \\
\theta_4 
\end{pmatrix} = -2\epsilon_+\epsilon_- \left( 1 - \frac{2\epsilon_-}{\epsilon_+} \right) \begin{pmatrix}
\theta_1 \\
\theta_2 \\
\theta_3 \\
\theta_4 
\end{pmatrix} 
\] (3.7.17)

which clearly has strictly negative Lyapunov exponents up to this order of expansion.

3.7.2 Resolving the Fixed Line in the U(2) Symmetric Case

The flow diagram in Fig. 3.7, obtained by perturbation theory to quadratic order in the interactions, suitably describes the transport physics of single-electron-tunneling phases for most ranges of infinitesimal interactions \(\epsilon_+\) and \(\epsilon_-\). However, when \(\epsilon_- = 0\), Eqs. (3.4.13) become symmetric under arbitrary U(2) transformations in band index space and describe a fixed line \(T_0 + T_\pi = 1\). In this appendix, we use bosonization at the \(T_0 = 1, T_\pi = 0\) “M-phase” fixed point to determine whether this fixed line is a genuine physical phenomenon or an artifact of our \(\mathcal{O}(\epsilon_\pm^2)\) perturbation theory. The first section of this appendix details the derivation of a Euclidean action about an M fixed point, working from the action for the fully-open CC phase. The second section utilizes that action to calculate flow equations beyond quadratic order in the vicinity of the M phase, resolving the fixed line to additional fixed points for weak-to-moderate interactions.
3.7.2.1 Deriving the Euclidean Action for the $T_0 = 1, T_\pi = 0$ M-Phase Fixed Point

To examine the higher-order behavior of tunneling processes about the $T_0 = 1, T_\pi = 0$ corner fixed point in Eq. (3.4.13), we have to first obtain a theory for that fixed point in terms of our existing theory for the $T_{0,\pi} = 1$, fully-open fixed point. As we will be focusing on the fate of the quadratic-order fixed line at $g_- = 1$, we will for the purposes of this calculation specialize to $g_+ = g, g_- = 1$. Integrating out the $\phi_{+/-,c/s,\rho/v}$ sectors in Eq. (3.3.17), we can propose as a starting point the Euclidean action about the CC fixed point:

$$S_{CC} = \frac{1}{4\pi\beta} \sum_{\alpha = c,s} \sum_{\omega_n} |\omega_n| \tilde{\theta}_\alpha^T g_\alpha \tilde{\theta}_\alpha^v$$  \hspace{1cm} (3.7.18)

where

$$\tilde{\theta}_\alpha^v = \begin{pmatrix} \theta_{+\alpha}\rho \\ \theta_{+\alpha}v \\ \theta_{-\alpha}\rho \\ \theta_{-\alpha}v \end{pmatrix},$$  \hspace{1cm} (3.7.19)
We can introduce weak tunneling processes,

\[
V_{0/\pi} = \frac{v_{0/\pi}}{2} \left[ \psi_{0/\pi,RK}^{\dagger} \psi_{0/\pi,LK} + K \leftrightarrow K' + \uparrow \leftrightarrow \downarrow + H.C. \right] \\
= v_{0/\pi} \sum_{\sigma,u} \cos (\theta_{0/\pi,\sigma u})
\]

(3.7.21)

where \( \sigma = \uparrow, \downarrow \) and \( u = K, K' \).

These processes will generally be present within the vicinity of the \( T_0 = T_{\pi} = 1 \) fixed point. Both of these processes are just single-electron tunneling, so as described in 3.3.2, they are marginal or irrelevant (\( \Delta(v_0) = \Delta(v_\pi) = \frac{1}{8}[g + 1/g + 6] \)) for all values of \( g \), such that we may arbitrarily increase the coupling strength \( v_{0/\pi} \) without new, additional tunneling processes becoming relevant. Respecting time-reversal, valley-index, and band-index symmetries, \( V_{0/\pi} \) are restricted to live in the plane of Fig. 3.8 and therefore turning up \( v_{0/\pi} \) represents motion away from the CC fixed point along the \( T_{0/\pi} \) axes respectively.
For this reason, we need to return $S_{CC}$ to the $0, \pi$ basis so that we can generate an M phase action by taking the tunneling strength $v_\pi \to \infty$ and “pinch off” just the $\pi$ band. Additionally, we will find it easier to work in a basis for which the tunneling operators $V_{0/\pi}$ are just sums of cosines. From our bosonization work in 3.3 and utilized earlier in this appendix, we recall that $\theta_{\pm \sigma u} = \theta_{0 \sigma u} \pm \theta_{\pi \sigma u}$. We will also need to transform valley indexes utilizing the property that $\theta_{a \sigma, K/K'} = \theta_{a \sigma \rho} \pm \theta_{a \sigma v}$ where $a = 0, \pi$. Combining these definitions, we create the unitary change-of-basis

$$\vec{\theta}_\alpha^v = \begin{pmatrix} \theta_{+ \alpha \rho} \\ \theta_{+ \alpha v} \\ \theta_{- \alpha \rho} \\ \theta_{- \alpha v} \end{pmatrix} = \mathbb{Y} \begin{pmatrix} \theta_{0 \alpha K} \\ \theta_{0 \alpha K'} \\ \theta_{\pi \alpha K} \\ \theta_{\pi \alpha K'} \end{pmatrix} = \mathbb{Y} \vec{\theta}_\alpha$$ (3.7.22)

where $\alpha = c, s$ and

$$\mathbb{Y} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$ (3.7.23)

and we can note that $\mathbb{Y}^T = \mathbb{Y}^{-1} = \mathbb{Y}$. Under this transformation, the action becomes
$$S_{CC} = \frac{1}{4\pi\beta} \sum_{\alpha=c,s} \sum_{\omega_n} |\omega_n| \vec{\theta}_\alpha^r \gamma_\alpha \gamma_\bar{\alpha}$$  \hspace{1cm} (3.7.24)$$

where $\gamma_\alpha \gamma$ separates into blocks:

$$\gamma_\alpha \gamma = \frac{1}{4} \begin{pmatrix} A & B \\ B & A \end{pmatrix}$$  \hspace{1cm} (3.7.25)$$

where

$$A = \begin{pmatrix} g + \frac{1}{g} + 2 & g - \frac{1}{g} \\ g - \frac{1}{g} & g + \frac{1}{g} + 2 \end{pmatrix} = (g + 1/g + 2) \mathbb{I} + (g - 1/g) \sigma^x$$

$$B = \begin{pmatrix} g + \frac{1}{g} - 2 & g - \frac{1}{g} \\ g - \frac{1}{g} & g + \frac{1}{g} - 2 \end{pmatrix} = (g + 1/g - 2) \mathbb{I} + (g - 1/g) \sigma^x = A - 4 \mathbb{I}. \hspace{1cm} (3.7.26)$$

As the spin sector is noninteracting, $\gamma_\alpha \gamma = \mathbb{I}$.

To complete the transformation into the basis of
\[ V_{CC} = V_0 + V_\pi, \quad (3.7.27) \]

we now need to address the spin degree of freedom. Utilizing the definitions of the spin and charge sectors (Eqs. (3.3.6)),

\[
\begin{pmatrix}
\vec{\theta}_c \\
\vec{\theta}_s
\end{pmatrix}
= \begin{pmatrix}
I & I \\
I & -I
\end{pmatrix}
\begin{pmatrix}
\vec{\theta}_\uparrow \\
\vec{\theta}_\downarrow
\end{pmatrix}.
\quad (3.7.28)
\]

Applying this to our action, we can complete this change of basis:

\[
S_{CC} = \frac{1}{4\pi\beta} \sum_{\omega_n} |\omega_n| \left( \begin{pmatrix}
\vec{\theta}_\uparrow \\
\vec{\theta}_\downarrow
\end{pmatrix}
\right)
\begin{pmatrix}
Y_{g_c}Y + I & Y_{g_c}Y - I \\
Y_{g_c}Y - I & Y_{g_c}Y + I
\end{pmatrix}
\begin{pmatrix}
\vec{\theta}_\uparrow \\
\vec{\theta}_\downarrow
\end{pmatrix}.
\quad (3.7.29)
\]

The most general action, to first order in irrelevant electron tunneling processes, is then:

\[
S = S_{CC} + \int_{\tau_C}^{\beta} \frac{d\tau}{\tau_C} V_{CC}.
\quad (3.7.30)
\]

To drive towards the \( T_0 = 1, T_\pi = 0 \) fixed point, we need only take \( v_\pi \to \infty \), as we have already established \( v_0 \) and \( v_\pi \) as the quantities which push back along the
and $T_\pi$ axes respectively.

To massage something useful out of this strong-tunneling limit, we can utilize an extreme limit of the Villain approximation, following procedurally a longer formulation of the Kane-Fisher problem [105]. Note that the partition function is the product of the contribution from $S_{CC}$ and a term of the form $e^{-v_\pi \int d\tau \cos \theta}$. As $v_\pi \to \infty$, the entire partition function is zeroed out except when $\cos \theta$ is a minimum. Acknowledging this, one can make the substitution of $e^{-v_\pi \int d\tau \cos \theta} \to \sum_m e^{im\theta}$ where $m$ is now a discrete step in time. The partition function can then be integrated over $\theta$ once we complete the square to give a new Gaussian effective action in terms of the integer $m$. Now, we can define $m = \partial_\tau \varphi / 2\pi$, such that in the frequency domain, our bare action has the same form and an inverse Luttinger parameter. Hopping events between the minima of $\cos \theta$ are instantons whose term in the action takes the form $t \int d\tau \cos \varphi$, the same as if we had defined our electron operators as exponentials of $\varphi$ fields and examined tunneling about the bare action. This equivalence between strong electron tunneling in $\theta$ and weak quasiparticle backscattering in $\varphi$ is a key feature of the Kane-Fisher problem for single-impurity scattering in Luttinger liquids. Its physical implications, as well as a much more detailed derivation of it, can be found in Ref. 105.

For four-terminal quantum point contacts, however, this equivalence manifests itself as a relationship between strong left-to-right electron tunneling and weak top-to-bottom electron backscattering [199]. Therefore, our ultimate goal is to arrive
at \( \varphi \) operators which correspond to the \( t_{\pi \to \pi} \) single-particle tunneling processes in Fig. 3.3 about an M point in Fig. 3.8, for which only the \( \pi \) band is pinched off.

In our problem, the result of taking \( v_{\pi} \to \infty \) and utilizing this trick is a fair bit more complicated due to the larger set of operators in the action and the matrix nature of the interactions.

First, let us start by reducing this problem into manageable blocks. We can simplify using the following definitions:

\[
\Upsilon_g Y \pm l = U_\pm = \frac{1}{4} \begin{pmatrix} A \pm 4I & B \\ B & A \pm 4I \end{pmatrix} = \frac{1}{4} \begin{pmatrix} A_\pm & B \\ B & A_\pm \end{pmatrix} \tag{3.7.31}
\]

such that now

\[
S_{CC} = \sum_{\omega_n} \frac{|\omega_n|}{4\pi \beta} \left[ \sum_{\sigma=\uparrow,\downarrow} \bar{\theta}_\sigma U_+ \bar{\theta}_\sigma + 2\bar{\theta}_\uparrow U_- \bar{\theta}_\downarrow \right] \tag{3.7.32}
\]

where

\[
U_\pm = \Upsilon_g Y \pm l. \tag{3.7.33}
\]

As addressed in Eq. (3.7.30), the full action contains contributions from \( S_{CC} \)
as well as perturbative tunneling terms. To push towards the corner M phase, we can increase \( v_\pi \) greatly until it becomes valid to replace that part of the partition function with discrete delta functions in \( \tilde{\theta}_{\pi\sigma} \):

\[
\int_0^\beta \frac{d\tau}{\tau_c} V_{CC} = 2i \sum_{\sigma=\uparrow,\downarrow} \bar{m}_{\pi\sigma} \tilde{\theta}_{\pi\sigma} + \int_0^\beta \frac{d\tau}{\tau_c} [V_0 + T_\pi] \quad (3.7.34)
\]

\[
\tilde{\theta}_{\alpha\sigma} = \begin{pmatrix}
\theta_{\alpha\sigma K} \\
\theta_{\alpha\sigma K'}
\end{pmatrix}
\]

\[
(3.7.35)
\]

such that \( \tilde{\theta}_\sigma = \tilde{\theta}_{0\sigma} \oplus \tilde{\theta}_{\pi\sigma} \). \( T_\pi \) is an instanton tunneling term which enforces the condition that \( m_{a\sigma K/K'} \) is an integer. The factor of 2 in front of it is a normalization requirement from the \( c,s \rightarrow \uparrow,\downarrow \) change of basis. As described earlier, we can recognize the \( m_{a\sigma K/K'} \) as discrete steps in time of a new field:

\[
\bar{m}_{\pi\sigma} = \begin{pmatrix}
\bar{m}_{\pi\sigma K} \\
\bar{m}_{\pi\sigma K'}
\end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix}
\partial_t \varphi_{\pi\sigma K} \\
\partial_t \varphi_{\pi\sigma K'}
\end{pmatrix} = \frac{i\omega}{2\pi} \begin{pmatrix}
\varphi_{\pi\sigma K} \\
\varphi_{\pi\sigma K'}
\end{pmatrix} = \frac{i\omega}{2\pi} \tilde{\varphi}_{\pi\sigma}. \quad (3.7.36)
\]

Combining all of these definitions, we arrive at a full expression for the action
which has both $\theta$ and $\varphi$ fields in it:

\[
S = \left\{ \sum_{n} \frac{|\omega_n|}{16\pi\beta} \left[ \sum_{\sigma=\uparrow,\downarrow} \left( \sum_{a=0,\pi} \theta_{a\sigma} A_{a\sigma} T + 2\theta_{1\sigma} B \theta_{0\sigma} \right) \right] + 2 \sum_{a=0,\pi} \theta_{a\uparrow} A_{a\uparrow} \theta_{a\downarrow} + 2\theta_{0\uparrow} B \theta_{0\downarrow} \right) + 2 \sum_{a=0,\pi} \theta_{a\downarrow} A_{a\downarrow} \theta_{a\uparrow} + 2\theta_{0\downarrow} B \theta_{0\uparrow} \right) + 16i \text{sgn}(\omega_n) \sum_{\sigma=\uparrow,\downarrow} \tilde{\varphi}_{1\sigma} \theta_{1\sigma} \right) \right\} + \int_{0}^{\beta} \frac{d\tau}{\tau_c} \left[ V_0 + T_\pi \right] (3.7.37)
\]

where we have frequently exploited that $A_{\pm}$ and $B$ are symmetric.

After a good bit of algebra, we can complete the square twice here and integrate out the $\tilde{\theta}_{\pi\sigma}$, leaving us with an intermediate action $S_M$ about the $T_0 = 1$, $T_\pi = 0$ M-phase stable fixed point:

\[
S = S_M + \int_{0}^{\beta} \frac{d\tau}{\tau_c} V_M (3.7.38)
\]

\[
S_M = \frac{1}{4\pi\beta} \sum_{\omega_n} \left[ \left( \begin{array}{c} \tilde{\theta}_{0\uparrow} \\ \tilde{\theta}_{0\downarrow} \\ \varphi_{\pi\uparrow} \\ \varphi_{\pi\downarrow} \end{array} \right) S_M \left( \begin{array}{c} \tilde{\theta}_{0\uparrow} \\ \tilde{\theta}_{0\downarrow} \\ \varphi_{\pi\uparrow} \\ \varphi_{\pi\downarrow} \end{array} \right) \right] (3.7.39)
\]
\[ V_M = \sum_{\sigma, u} v_0 \cos (\theta_{0\sigma u}) + t_{\pi} \cos (\varphi_{\pi\sigma u}) \]  (3.7.40)

where \( \sigma = \uparrow, \downarrow; u = K, K'; \) and

\[
g_M = \begin{pmatrix}
2I + \alpha\sigma^x & \alpha\sigma^x & -\text{sgn}(\omega_n)\alpha\sigma^x & -\text{sgn}(\omega_n)\alpha\sigma^x \\
\alpha\sigma^x & 2I + \alpha\sigma^x & -\text{sgn}(\omega_n)\alpha\sigma^x & -\text{sgn}(\omega_n)\alpha\sigma^x \\
\text{sgn}(\omega_n)\alpha\sigma^x & \text{sgn}(\omega_n)\alpha\sigma^x & 2I - \alpha\sigma^x & -\alpha\sigma^x \\
\text{sgn}(\omega_n)\alpha\sigma^x & \text{sgn}(\omega_n)\alpha\sigma^x & -\alpha\sigma^x & 2I - \alpha\sigma^x \\
\end{pmatrix}, \quad \alpha = \frac{g - 1}{g + 1} \]  (3.7.41)

in which the sign on the bottom right block of \( g_M \) is owed to one of the sets of bosonic fields being evaluated at \(-\omega_n\) and the other at \(+\omega_n\). The tunneling term \( t_{\pi} \) for the \( \varphi \) fields represents weak, left-to-right tunneling of electrons with band index \( \pi \); making it very large would return the system back to the CC corner fixed point.

Correlation functions about this theory can be calculated using elements of the inverse of this matrix:
\[ 2g_{M}^{-1} = \frac{1}{2} \begin{pmatrix} 2\| - \alpha\sigma^{x} & -\alpha\sigma^{x} & \text{sgn}(\omega_{n})\alpha\sigma^{x} & \text{sgn}(\omega_{n})\alpha\sigma^{x} \\ -\alpha\sigma^{x} & 2\| - \alpha\sigma^{x} & \text{sgn}(\omega_{n})\alpha\sigma^{x} & \text{sgn}(\omega_{n})\alpha\sigma^{x} \\ -\text{sgn}(\omega_{n})\alpha\sigma^{x} & -\text{sgn}(\omega_{n})\alpha\sigma^{x} & 2\| + \alpha\sigma^{x} & \alpha\sigma^{x} \\ -\text{sgn}(\omega_{n})\alpha\sigma^{x} & -\text{sgn}(\omega_{n})\alpha\sigma^{x} & \alpha\sigma^{x} & 2\| + \alpha\sigma^{x} \end{pmatrix} \tag{3.7.42} \]

where the factor of 2 again comes from the spin-index change of basis and ensures that diagonal correlators like \( \langle e^{i\theta_{0}K(\tau)}e^{i\theta_{0}K(0)} \rangle \sim 1/\tau^{2} \) are appropriately marginal.

The calculations in the following section are also only appropriate provided that the single-particle, off-diagonal correlation functions are zero. This requirement is enforced for the \( \theta \) fields for \( 2 - \alpha > 1 \) and by \( 2 + \alpha > 1 \) for the \( \phi \) variables. However, the range \(-1 < \alpha < 1\) is satisfied by all physical values of \( g \). Therefore, the only bounds on the validity of the \( S_{M} \) theory are the regions in Fig. 3.4 for which many-body processes become relevant.

### 3.7.2.2 Cubic-Order Fixed Points about the M Phase for \( g_{-} \approx 1 \)

In this section, we will, using the \( S_{M} \) theory established in the previous section, develop quartic-order flow equations for \( v_{0} \) and \( t_{\pi} \) for \( g_{-} = 1, g_{+} = g \). After establishing the flow in those variables, we will relate \( v_{0} \) and \( t_{\pi} \) to \( T_{b/\pi} \) in Eq. (3.4.13). Expanding \( g = 1 + \epsilon_{+} \), we will develop the cubic-order corrections to Fig. 3.7 close to the M-phase fixed points and obtain the schematic phase diagram Fig. 3.8.
There are two sets of correlation functions for each coupling coefficient that we
must calculate and rescale to obtain flow equations, as indicated by the two non-
zero, off-diagonal elements for each operator and spin in $g_M$. For now, we will work
just with the $v_0$ renormalization and then use band-index-exchange and pinch-off
symmetries to relate them to the flow of $t_\pi$.

Starting with the $\theta_{\sigma \uparrow K}$ operator, we can calculate terms in the cumulant expan-
sion to cubic order:

$$
\delta v_0 = v_0^3 \sum_{\sigma=\uparrow,\downarrow} \int_{-\infty}^{\infty} d\tau_1 d\tau_2 \left[ \langle T_\tau \left[ e^{i\theta_{\sigma \uparrow K}(\tau)} e^{i\theta_{\sigma \uparrow K'}(\tau_1)} e^{-i\theta_{\sigma \uparrow K'}(\tau_2)} \right] \rangle - \langle e^{i\theta_{\sigma \uparrow K}(\tau)} \rangle \langle T_\tau \left[ e^{i\theta_{\sigma \uparrow K'}(\tau_1)} e^{-i\theta_{\sigma \uparrow K'}(\tau_2)} \right] \rangle \right] 
+ v_0 t_\pi^2 \sum_{\sigma=\uparrow,\downarrow} \int_{-\infty}^{\infty} d\tau_1 d\tau_2 \left[ \langle T_\tau \left[ e^{i\theta_{\sigma \uparrow K}(\tau)} e^{i\varphi_{\pi \sigma K'}(\tau_1)} e^{-i\varphi_{\pi \sigma K'}(\tau_2)} \right] \rangle - \langle e^{i\theta_{\sigma \uparrow K}(\tau)} \rangle \langle T_\tau \left[ e^{i\varphi_{\pi \sigma K'}(\tau_1)} e^{-i\varphi_{\pi \sigma K'}(\tau_2)} \right] \rangle \right].
$$

(3.7.43)

As before, $T_\tau$ is the time-ordered product and for each of the integrals, the second
term is the disconnected piece. Taking into account all possible time orderings, we
can rewrite this:
\[
\delta v_0 = 2v_0^3 \int_{-\infty}^{\infty} d\tau_1 d\tau_2 \frac{1}{\tau_{12}^2} \left[ \left( \frac{\tau_1}{\tau_2} \right)^\alpha - 1 \right] \\
+ 2v_0 t_\pi^2 \int_{-\infty}^{\infty} d\tau_1 d\tau_2 \frac{1}{\tau_{12}^2} \times \\
\left[ \Theta(\tau \not\in (\tau_1, \tau_2)) + e^{\pi i \alpha} \Theta(\tau_1 < \tau < \tau_2) + e^{-\pi i \alpha} \Theta(\tau_2 < \tau < \tau_1) - 1 \right]
\]

(3.7.44)

where \( \tau_{12} = \tau_1 - \tau_2 \) and \( \Theta(\tau, \tau_1, \tau_2) \) is the Heaviside step function expressed in conditional notation. These integrals can be performed analytically and, after a bit of work, we arrive at an explicit equation for \( \delta v_0 = v'_0 - v_0 \):

\[
\delta v_0 = \log b \left[ 4v_0^3 \pi \alpha \tan \left( \frac{\pi \alpha}{2} \right) - 8v_0 t_\pi^2 \sin^2 \left( \frac{\pi \alpha}{2} \right) \right]
\]

(3.7.45)

where \( b \) is the time-integral cutoff. Rescaling \( b \to be^{-l} \) and taking into account the flow equations’ invariance under combined exchange \( v_0 \leftrightarrow t_\pi, \alpha \leftrightarrow -\alpha \), we arrive at our higher-order flow equations:
\[
\frac{dv_0}{dl} = 4v_0^3\pi\alpha \tan\left(\frac{\pi\alpha}{2}\right) - 8v_0t_\pi^2 \sin^2\left(\frac{\pi\alpha}{2}\right),
\]
\[
\frac{dt_\pi}{dl} = 4t_\pi^3\pi\alpha \tan\left(\frac{\pi\alpha}{2}\right) - 8v_0^2t_\pi \sin^2\left(\frac{\pi\alpha}{2}\right) \tag{3.7.46}
\]

which are valid only in a perturbative vicinity of this M-phase fixed point and for weak-to-moderate interactions.

Now, to answer our initial question, we will examine the consequences of our new flow equations near the vicinity of the possible fixed line in Fig. 3.7b. Expanding \( g = 1 + \epsilon_+ \), \( \alpha^2 = \epsilon_+^2/4 \) such that Eq. (3.7.46) reduces to the \( \epsilon_- = 0 \) limit of Eq. (3.4.13) under the substitution:

\[
v_0 = \frac{2}{\pi} \sqrt{1 - T_0}, \quad t_\pi = \frac{2}{\pi} \sqrt{T_\pi}. \tag{3.7.47}
\]

when \( 1 - T_0 \ll 1, \ T_\pi \ll 1 \). We also know that the linear terms in \( dT_0/\pi/dl \) must agree with any local expansion in the \( T_0 - T_\pi \) plane, such that we can restore flow to linear order in \( \epsilon_- \) near the M-phase by extracting the leading term in Eq. (3.4.13):
\[
\frac{dT_0}{dl} \bigg|_{\mathcal{O}(\epsilon_+ \epsilon_-)} = 8\epsilon_+ \epsilon_- (1 - T_0)
\]
\[
\frac{dT_\pi}{dl} \bigg|_{\mathcal{O}(\epsilon_+ \epsilon_-)} = -8\epsilon_+ \epsilon_- T_\pi
\]

(3.7.48)

where we have used the same approximation \(1 - T_0 \ll 1, T_\pi \ll 1\). Combining this with an expansion of Eq. (3.7.46) to quartic order in \(\epsilon_+\), we obtain, finally, higher-order flow equations about an M-phase fixed point:

\[
\frac{d}{dl} (1 - T_0) = -8\epsilon_+ \epsilon_- (1 - T_0) + 4(1 - T_0)^2 \left[ \epsilon_+^2 + \frac{\pi^2 \epsilon_+^4}{48} \right] - 4(1 - T_0) T_\pi \left[ \epsilon_+^2 - \frac{\pi^2 \epsilon_+^4}{48} \right]
\]
\[
\frac{dT_\pi}{dl} = -8\epsilon_+ \epsilon_- T_\pi + 4 T_\pi^2 \left[ \epsilon_+^2 + \frac{\pi^2 \epsilon_+^4}{48} \right] - 4(1 - T_0) T_\pi \left[ \epsilon_+^2 - \frac{\pi^2 \epsilon_+^4}{48} \right].
\]

(3.7.49)

Equation (3.7.2.2) contains a few points of interest. First and foremost, it reflects the pinch-off symmetry in its invariance under the exchange \((1 - T_0) \leftrightarrow T_\pi\). It also contains fixed points at \(T_0 = 1 - \frac{2\epsilon_-}{\epsilon_+}\), \(T_\pi = 0\) and at \(T_0 = 0\), \(T_\pi = \frac{2\epsilon_-}{\epsilon_+}\), in agreement with the small \(\epsilon_-/\epsilon_+\) limit of Fig. 3.7. We specifically normalized our correlations about \(S_M\) to fix this agreement, such that we could locate at quartic order in \(\epsilon_+\) any local quantum critical points which control the transition between the CC/II and M phases.
On the line $1 - T_0 = T_\pi$, Eq. (3.7.2.2) admits an additional fixed point at

$$1 - T_0 = T_\pi = \frac{48 \epsilon_-}{\pi^2 \epsilon_+^3},$$

(3.7.50)

relevant flow lines from this point head off towards the central $T_0 = T_\pi = 1/2$ critical point, even in the $\epsilon_- = 0$ case when this point converges with the other critical points at the corner. Therefore, this point stands as a demonstration that the fixed line in Fig. 3.7b is an artifact of $\mathcal{O}(\epsilon_+^2)$ perturbation theory, at least in the vicinity of the $T_0 = 1, T_\pi = 0$ M point. It is most likely that this flow away from the M point continues, to lowest order, all the way to the central quantum critical point. This infers that the phase diagram of this system for weak-to-moderate interactions is best described by the schematic Fig. 3.8.
Part II

Topology and Geometry in Nodal Materials
Chapter 4

Dirac Line Nodes in Inversion-Symmetric Crystals with Weak Spin-Orbit Coupling

4.1 Abstract

We propose and characterize a new $\mathbb{Z}_2$ class of topological semimetals with a vanishing spin–orbit interaction. The proposed topological semimetals are characterized by the presence of bulk one-dimensional (1D) Dirac Line Nodes (DLNs) and two-dimensional (2D) nearly-flat surface states, protected by inversion and time–reversal symmetries. We develop the $\mathbb{Z}_2$ invariants dictating the presence of DLNs based
on parity eigenvalues at the parity–invariant points in reciprocal space. Moreover, using first-principles calculations, we predict DLNs to occur in Cu$_3$N near the Fermi energy by doping non-magnetic transition metal atoms, such as Zn and Pd, with the 2D surface states emerging in the projected interior of the DLNs. This chapter includes a brief discussion of the effects of spin–orbit interactions and symmetry-breaking as well as comments on experimental implications. \textit{This chapter originally appeared as an article by Youngkuk Kim, Benjamin J. Wieder, C. L. Kane, and Andrew M. Rappe in Physical Review Letters in 2015 [112].}

### 4.2 Introduction

A recent development in condensed matter physics has been the discovery of semimetallic features in electronic band structures protected by the interplay of symmetry and topology. A tremendous amount of progress has been made in materials with strong spin–orbit interactions, such as the surface states of topological insulators [83, 171] and topological crystalline insulators [60], as well as the gapless bulk states of Weyl and Dirac semimetals [191, 209, 244]. Related topological phenomena can occur in materials with vanishing (or weak) spin–orbit interactions [8]. Indeed, the prototypical topological semimetal is graphene [35], which exhibits Dirac points that are robust to the extent that the spin–orbit interaction in carbon is weak. In the absence of spin–orbit interactions, the Dirac points in graphene are topologically protected by the combination of inversion and time–reversal symmetries.
In this chapter we study a related phenomenon for three dimensional (3D) materials with weak spin–orbit interaction. We show that the combination of inversion and time–reversal symmetries protects Dirac line nodes (DLNs), for which the conduction band and valence band meet along a line in momentum space, and we predict realistic materials in which they should occur. DLNs have been discussed previously in the context of models that have an additional chiral symmetry, which can arise on a bipartite lattice with only nearest neighbor hopping. In this case, the DLN can be constrained to occur at zero energy. However, chiral symmetry is never expected to be an exact symmetry of a band structure. We will show that despite the absence of chiral symmetry, the line node is protected, though it is not constrained to sit at a constant energy. We will show, however, that in the vicinity of a band inversion transition, a DLN can occur in the form of a small circle, whose energy is approximately flat. The presence of such a Dirac circle has interesting consequences for the surface states, and we show that on the projected interior of the Dirac circle, the surface exhibits a nearly flat band, which must be half–filled when the surface is electrically neutral. Such surface states could be an interesting platform for strong correlation physics. We introduce a class of materials and use first–principles density functional theory (DFT) calculations to show that they can be tuned through the band inversion transition and exhibit the predicted Dirac circle, as well as a more complex nodal structure. A similar DLN near an inversion transition has recently been predicted in a 3D graphene network [207, 220]. Recently, DLNs also have been proposed in systems with strong spin-orbit inter-
actions, such as perovskite irridates [39, 111] and non-centrosymmetric semimetals [219], but in those systems the mechanism of symmetry protection is different.

We will begin by elucidating the topological constraints that inversion and time-reversal symmetries impose. We will then introduce a $\mathbb{Z}_2$ topological invariant (related to the invariant characterizing a 3D topological insulator) which signifies the presence of DLNs. We will then present DFT calculations on transition metal–doped Cu$_3$N that predict a Dirac circle, as well as nearly-flat boundary modes. We will then introduce a simple low–energy $k \cdot p$ model that explains the appearance of the Dirac circle at a band inversion, and allows for a simple description of the resulting boundary modes.

### 4.3 Topological Protection of Line Nodes under $\mathcal{I}$ and $\mathcal{T}$

Consider a 3D Bloch Hamiltonian $\mathcal{H}(\mathbf{k})$ that is invariant under inversion $\mathcal{I}$ and time-reversal $\mathcal{T}$. In the absence of spin–orbit interactions we may consider $\mathcal{T}^2 = +1$. The occupied Bloch eigenstates are characterized by a Berry connection $\mathbf{A}(\mathbf{k}) = -i \sum_n \langle u_n(\mathbf{k}) | \nabla_\mathbf{k} u_n(\mathbf{k}) \rangle$. $\mathcal{I}$ and $\mathcal{T}$ symmetries constrain the Berry phase, $\omega(C) = \exp i \oint_C \mathbf{A} \cdot d\mathbf{k}$, on any closed loop $C$ in momentum space, to satisfy $\omega(C) = \omega(-C)$ and $\omega(C) = \omega(-C)^*$, respectively. It follows that loops $C$ are characterized by a $\mathbb{Z}_2$ topological invariant $\omega(C) = \pm 1$. The non–trivial loops $\omega(C) = -1$ must

\[ \text{Since } [\mathcal{H}(\mathbf{k}), \mathcal{I}\mathcal{T}] = 0, \text{ this } \mathbb{Z}_2 \text{ invariant can also be understood as characterizing one parameter families of Hamiltonians in class AI [200]} \]
enclose a degeneracy. In two dimensions, this explains the symmetry protection of the Dirac points in graphene. In three dimensions, it guarantees that a line of degeneracies must pierce any surface bounded by $C$.

The parity eigenvalues $\xi_n(\Gamma_a) = \pm 1$ of the occupied Bloch states at the 8 parity-invariant momenta $\Gamma_a$ provide an important constraint that allows us to identify topologically protected line nodes. First, consider a time-reversal invariant loop $C_{ab} = c_{ab} - \bar{c}_{ab}$ that connects $\Gamma_a$ and $\Gamma_b$ along two time-reversed paths $c_{ab}$ and $\bar{c}_{ab}$. In the supplementary material we prove that the Berry phase on this loop satisfies

$$\omega(C_{ab}) = \xi_a \xi_b; \quad \xi_a = \prod_n \xi_n(\Gamma_a). \quad (4.3.1)$$

If we now consider four parity-invariant points, the contour $C_{ab} - C_{cd}$ defines the boundary $\partial S_{abcd}$ of a surface $S_{abcd}$ in momentum space. The Berry phase on $\partial S_{abcd}$ counts the number of DLNs $N(S_{abcd})$ that pierce that surface. We thus conclude that

$$(-1)^{N(S_{abcd})} = \xi_a \xi_b \xi_c \xi_d. \quad (4.3.2)$$

Thus, when $\xi_a \xi_b \xi_c \xi_d = -1$ there must be an odd number of DLN piercing any surface $S_{abcd}$, with the simplest case being just a single one. This relation is quite similar to the topological invariants $(\nu_0; \nu_1 \nu_2 \nu_3)$ characterizing a (strong or weak) $\mathbb{Z}_2$ topological insulator in the presence of spin–orbit interactions [61, 65]. Indeed, in a topological insulator with $\xi_a \xi_b \xi_c \xi_d = -1$, when the spin–orbit interaction is turned off a DLN must appear, because the system can not be adiabatically connected to
This connection to the parity eigenvalues suggests a route towards realizing the DLNs: Starting with a trivial insulator, invert a pair of opposite-parity bands. At the inversion transition a small Dirac circle will necessarily emerge and grow. In the following we will predict a class of real materials which exhibits this behavior, and analyze the low–energy structures which emerge.

### 4.4 Line Nodes in Cu$_3$N

Searching for materials that consist of light elements and preserve $\mathcal{T}$ and $\mathcal{I}$ symmetries, we find that copper nitride, Cu$_3$N, a narrow–gap semiconductor ($E_g \sim 0.3$ eV) [104], fosters DLNs near the Fermi level via an insulator–to–metal transition driven by doping transition metal atoms. Copper nitride, first synthesized in 1937 [104], is stable in air at room temperature with a cubic anti–ReO$_3$ structure in space group 221 (Pm$\bar{3}$m). It contains a rather large void at the center of the cubic unit cell, as shown in Fig. 4.1. This void can host extrinsic atoms such as N [77], Li [76, 92], Pd [78, 100, 150, 186, 249], Rh, Ru [186], Zn, Ni, Cd [150], Cu [92, 149], Fe, Ti [52], Ag [169], La, Ce [230], as well as many other transition–metal atoms [45]. In particular Ni, Cu, Pd, An, Ag, and Cd [150] are found to drive an electronic transition in Cu$_3$N into a semimetal without breaking $\mathcal{T}$ symmetry [45], by which we expect that DLNs form near the Fermi energy.
Figure 4.1: Crystal structure of Cu$_3$NX. X represents a transition metal atom intercalated at the body-center of the cubic unit cell of Cu$_3$N in an anti-ReO$_3$ structure.

To demonstrate the existence of DLNs in the transition metal–doped Cu$_3$N, we perform first-principles calculations based on DFT. We employ the Perdew–Burke–Ernzerhof–type generalized gradient approximation [167] as implemented in the QUANTUM ESPRESSO package [72]. Norm-conserving, optimized, designed nonlocal pseudopotentials are generated by the OPIUM package [173, 175]. The wave functions are expanded in a plane-wave basis with an energy cutoff of 680 eV. We initially consider the spin–orbit interaction based on a scalar–relativistic pseudopotential [74], and later, we will discuss the effect of spin–orbit interactions, based on a fully-relativistic non–collinear scheme.

The low–energy electronic structures of Cu$_3$NX are more or less similar for X = \{Ni, Cu, Pd, An, Ag, Cd\}, as reported in Ref. [150]. Here we present the results of Cu$_3$NZn and Cu$_3$NPd as representatives of transition metal–doped Cu$_3$N systems. Note that these are extreme cases where the transition metal atoms are maximally
Figure 4.2: (color online) Electronic structures and $Z_2$ indices of (a) Cu$_3$NZn and (b) Cu$_3$NPd. Bands are drawn along the high-symmetry lines of the BZ (inset). The Dirac points are indicated by red circles. Parity eigenvalues are illustrated at the eight parity-invariant points in the first octant of the BZ.

doped. In Cu$_3$NZn the conduction and valence bands are mainly comprised of conduction $A_{2u}$ and valence $A_{1g}$ states near the Fermi energy. As shown in Fig. 4.2, these bands are inverted at the $X$ points, forming two-dimensional (2D) Dirac points on the $X$–$M$ and $R$–$X$ lines (enclosed by red circles in the figure). These Dirac points signal the presence of a DLN enclosing $X$. Although there are more degenerate points near the Fermi level, and bands crossing the Fermi energy near the $R$ point, we will simplify and here focus only on the bands near $X$. On the other hand, the conduction and valence bands of Cu$_3$NPd are comprised of $T_{2g}$ and $T_{1u}$ states, which are inverted at the $R$ point, forming the Dirac points on the $R$–$X$ and $M$–$R$ lines. These Dirac points are in fact parts of a DLN that encloses the $R$ point, as shown below.

\footnote{See the supplementary material for the discussion on the doping concentration.}
The nodal lines of the conduction and valence bands in the 3D BZ are shown in Fig. 4.3. As mentioned above, DLNs appear near the $X$ points in the Cu$_3$NZn system. The cubic symmetry of the system dictates three DLNs encircling the three inequivalent $X$ points $X^r = \pi \hat{r}/a$, where $r = x, y,$ and $z$. Similarly, Cu$_3$NPd also exhibits three DLNs due to the cubic symmetry, but since they appear enclosing the $R$ point, they form in a gyroscope shape. In both systems, the DLNs are contained in three mirror-invariant planes at $X^x$, $X^y$, and $X^z$, due to the corresponding mirror symmetries. We expect that breaking the mirror symmetries should unlock the DLNs from the mirror planes, but that the DLNs will survive as they are protected by $\mathcal{I}$ and $\mathcal{T}$.

The appearance of DLNs agrees with the topological prediction of $Z_2$ invariants $(\nu_0; \nu_1\nu_2\nu_3)$, calculated from the parity analysis. In Cu$_3$NZn, parities at the eight time-reversal invariant momenta ($\Gamma, 3X, 3M, R$) give $(\nu_0; \nu_1\nu_2\nu_3) = (1; 111)$, which dictates that there should be DLNs threading half the invariant plane at $X^r = \pi \hat{r}/a$ ($r = x, y, z$) an odd number of times. The three DLNs enclosing the $X$ points fulfill this topological constraint (see the supplementary material for more details of this analysis). Similarly, in Cu$_3$NPd we find that $(\nu_0; \nu_1\nu_2\nu_3) = (1; 111)$, which is also in accordance with the formation of the three DLNs enclosing $R$. In this case, each invariant plane at $X^r$ is threaded three times by all three DLNs.

A low–energy $\bm{k} \cdot \bm{p}$ Hamiltonian describing the conduction $A_{2u}$ and valence $A_{1g}$ states, which form the DLNs in Cu$_3$NZn, captures the essential features of the
Figure 4.3: (color online) Dirac line nodes in the Brillouin Zone (BZ). (a) and (b) Cu$_3$NZN, and (c) and (d) Cu$_3$NPd. The DLNs are illustrated by red curves in the 3D BZ [(a) and (c)] and on the 2D boundary plane of the BZ at $k = X^r$ [(b) and (d)].

DLNs. Near $X^r$, symmetries dictate a two–band Hamiltonian

$$
H_r = (\bar{\epsilon} + a_\perp |q_\perp|^2 + a_r q_r^2) \mathbb{1}_r + v q_r \tau^y + (\Delta \epsilon + b_\perp |q_\perp|^2 + b_r q_r^2) \tau^z,
$$

(4.4.1)

where $q = k - X^r$, $\perp$ represents the normal components to $\hat{r}$, and the Pauli matrices $\{\mathbb{1}_r, \tau^i\}$ describe the $A_{1g}$ and $A_{2u}$ states. The form of $H_r$ is uniquely determined by inversion $I = \tau^z$ and time–reversal $T = K$ ($K$ being complex conjugation), together with the $D_{4h}$ point group symmetries of $X$. It gives energy eigenvalues

$$
E_{\pm}(q) = \bar{\epsilon} + a_\perp |q_\perp|^2 + a_r q_r^2
$$

$$
\pm \sqrt{(\Delta \epsilon + b_\perp |q_\perp|^2 + b_r q_r^2)^2 + v^2 q_r^4}.
$$

(4.4.2)
A DLN forms at \( q_r = 0 \) and \( |q_\perp|^2 \equiv q_0^2 = -\Delta/b_\perp \), when the bands are inverted \((\Delta \epsilon < 0)\). The DFT results determine \( \Delta \epsilon \sim -0.4 \text{ eV} \). In Cu\(_3\)NPd, unlike in Cu\(_3\)NZn, there are conduction \( T_{2g} \) and valence \( T_{1u} \) states, instead leading to a six–band Hamiltonian \( \mathcal{H} \). However, this can be decomposed into three copies of \( \mathcal{H}_r \) with \( r = x, y, \) and \( z \) and \( \mathcal{H} = \mathcal{H}_x \oplus \mathcal{H}_y \oplus \mathcal{H}_z \), giving rise to three gyroscope–shaped DLNs. Therefore, the essential features of the DLNs should be the same between Cu\(_3\)NZn and Cu\(_3\)NPd, aside from the former having a single DLN occurring in three inequivalent valleys of the BZ \((X \text{ points})\) and the latter having three DLNs in a single valley \((R \text{ point})\).

This model Hamiltonian also describes boundary modes. Consider a boundary perpendicular to \( \hat{r} \) in which \( \Delta \epsilon \) varies between a negative (inverted) value and a large positive value. Fixing \( q_\perp \) and considering the theory to linear order in \( q_r \to -i\partial_r \),

\[
\mathcal{H}_z(q) = -iv\tau^y \partial_r + (\Delta \epsilon(r) + b_\perp q_\perp^2)\tau^z + (\bar{\epsilon} + a_\perp q_\perp^2)\mathbb{1}_r. \tag{4.4.3}
\]

For each \( k_\perp \) this defines a Jackiw–Rebbi problem [98]. When \( \Delta \epsilon + b_\perp k_\perp^2 < 0 \) there will be a boundary mode at the surface. In general the boundary band is not flat, but disperses for \( k_\perp < k_F \)

\[
\epsilon_0(k_\perp) = \bar{\epsilon} + a_\perp k_\perp^2 \leq 0. \tag{4.4.4}
\]

If \( a = 0 \) however, the surface band is flat. This reflects an additional chiral symmetry \( \{\mathcal{H}, \tau^z\} = 0 \) at this point. In this model, the value of \( a \) is related to the
difference of the effective masses of the $A_{1g}$ and $A_{2u}$ bands. If the surface in the absence of inversion is electrically neutral, then after inversion the surface will be neutral when the surface band is half-filled. This leads to a narrow surface band, where electron density $q_0^2/4\pi = |\Delta \epsilon|/4\pi b_\perp$ is controlled by the degree of band inversion. In the absence of screening from other bands, this surface band will tend to be pinned at the Fermi energy.

To study the surface states in Cu$_3$NZn, we calculate the band structures of a slab geometry with 40 unit cells, exposing the (100) Cu$_2$N surfaces to vacuum. Our calculation from first principles predicts that nearly-flat surface states emerge in the interiors of projected DLNs connecting the Dirac nodes, as shown in Fig. 4.4. The slab band structure exhibits the weakly-dispersing surface states near $\bar{\Gamma}$ in the projected interior of the DLN. The topological surface states resulting from closed DLNs are half-filled and nearly flat, providing a unique venue for interesting
strong-correlation and transport physics.

The strong spin–orbit interaction can induce diverse topological phases in DLN semimetals, including topological insulators, 3D Dirac semimetals [213, 244], or even other DLN semimetals [39]. Analogously to graphene, spin–orbit interaction can gap out DLNs and drive the system to a topologically-insulating phase. The resultant topological insulator should have the same topological $Z_2$ indexes as the DLN semimetal from which it originated. More interestingly, an additional crystalline symmetry may protect a part of the DLN in a symmetry-invariant region of the BZ, resulting in topological Dirac semimetals or crystalline symmetry–protected DLNs with strong spin–orbit interactions. We have tested the effect of spin–orbit interaction in Cu$_3$NPd using a fully-relativistic non–collinear scheme, and indeed found that $C_4$ symmetry along the $R$–$M$ line protects the Dirac point on the line, while the spin–orbit coupling otherwise opens a gap (with maximum size of $\sim 62$ meV on the $R$–$X$ line), thus giving rise to a 3D Dirac semimetal phase in a strong spin–orbit interacting regime. Note that Cu$_3$NPd is an extreme case where Pd is maximally doped, and thus the spin–orbit interactions due to Pd 4$d$ states are maximized. The spin–orbit interaction can be controlled either by the Pd–doping concentration, or by doping other group-X transition-metal atoms, such as Ni, Pd, and Pt. We thus expect both the DLN semimetal and 3D Dirac semimetal phases should be accessible in the Cu$_3$N system.
4.5 Chapter Acknowledgments

While this manuscript reproduced in this chapter was in the final stages of preparation we learned of recent work proposing DLNs in Ca$_3$P$_2$ [232]. YK acknowledges support from NSF grant DMR–1120901. CLK acknowledges support from a Simons Investigator grant from the Simons Foundation. AMR acknowledge support from the DOE Office of Basic Energy Sciences, under grant number DE–FG02–07ER15920. Computational support is provided by the HPCMO of the U.S. DOD and the NERSC of the U.S. DOE.

4.6 Supplemental Material

4.6.1 Proof of Eqn 4.3.1

Here we prove that the path integral of a Berry connection \( A(k) = -i \sum_n \langle u_n(k) | \nabla_k u_n(k) \rangle \)

\[ \omega(C_{ab}) = e^{i \oint_{C_{ab}} A \cdot dk} \quad (4.6.1) \]

on a loop \( C_{ab} = c_{ab} - \bar{c}_{ab} \) that connects two parity– and time–reversal–invariant points \( \Gamma_a \) and \( \Gamma_b \) along the two time–reversal paths \( c_{ab} \) and \( \bar{c}_{ab} \) (See Fig. 4.5) can be obtained by the parity eigenvalues \( \xi_n(\Gamma_a) = \pm 1 \) of the occupied Bloch states at
parity–invariant momenta $\Gamma_a$

$$\omega(C_{ab}) = \xi_a \xi_b; \quad \xi_a = \prod_n \xi_n(\Gamma_a). \quad (4.6.2)$$

It follows that

$$\omega(C_{ab}) = e^{i\int_a^b A(k) \cdot dk} e^{i\int_b^a A(k) \cdot dk} = e^{i\int_a^b (A(k) - A(-k)) \cdot dk}. \quad (4.6.3)$$

Inversion symmetry ($\mathcal{I}$) guarantees that $\langle u_n(-k) \rangle = e^{i\beta_n(k)} \mathcal{I} \langle u_n(k) \rangle$. It then follows that $A(k) - A(-k) = \nabla_k \sum_n \beta_n(k)$, so that

$$\omega(C_{ab}) = e^{i\sum_n \beta_n(\Gamma_b) - \beta_n(\Gamma_a)}. \quad (4.6.4)$$

Now consider $P(k) = \prod_n \langle u_n(-k) | \mathcal{I} | u_n(k) \rangle = e^{-i\sum_n \beta_n(k)}$. For a parity–invariant point $\Gamma_i$, $P(\Gamma_i) = \prod_n \xi_n(\Gamma_i)$, where $\xi_n(\Gamma_i) = \langle u_n(\Gamma_i) | \mathcal{I} | u_n(\Gamma_i) \rangle$ is the parity eigenvalue. We thus prove Eqn. (4.6.2).
4.6.2 $\mathbb{Z}_2$ topological invariants and Dirac line nodes of Cu$_3$NZn

The topological invariant $\xi_a \xi_b \xi_c \xi_d = -1$ dictates that for any invariant surface $S_{abcd}$ of the BZ, hosting four invariant momenta $\Gamma_i$ ($i = a, b, c, d$), there will be an odd number of Dirac line nodes (DLNs) intersecting the half surface at $k$ (and the other half at $-k$). Here we show that the DLNs that appear in Cu$_3$NZn satisfy this topological constraint. The cubic BZ of Cu$_3$NZn has eight distinct invariant momenta ($\Gamma, 3X, 3M, R$), and the parity eigenvalues at the high–symmetry momenta are calculated as $(\xi(\Gamma), \xi(X), \xi(M), \xi(R)) = (1, -1, 1, 1)$ as shown in Fig 4.6. Similar to the $\mathbb{Z}_2$ topological invariants of topological insulators [65], $\mathbb{Z}_2$ topological invariants
Figure 4.7: Dirac line nodes (DLNs) and invariant planes in the BZ of Cu$_3$NZn. Red circles represent the DLNs. The grey–shaded planes illustrate the invariant planes that the DLN at $\Gamma_3$ point ($L_3$) intersects, one of which ($S_{3567}$) is nontrivial and the other two ($S_{0235}$ and $S_{0136}$) are trivial. The intersecting position is depicted by red scheme on the planes.

$(\nu_0; \nu_1 \nu_2 \nu_3)$ can be defined in the DLN semimetals as

$$(-1)^{\nu_0} = \prod_{n_j=0,1} \xi_{n_1 n_2 n_3}, \quad (4.6.5)$$

$$(-1)^{\nu_i=1, 2, 3} = \prod_{n_j \neq i=0,1} \xi_{n_1 n_2 n_3}, \quad (4.6.6)$$

where $\xi_{i=(n_1 n_2 n_3)}$ are parity eigenvalues at the eight invariant momenta, $\Gamma_i=(n_1 n_2 n_3) = (n_1 b_1 + n_2 b_2 + n_3 b_3)/2$, with $n_j = 0, 1$, and the primitive reciprocal lattice vectors $b_i$. The $\mathbb{Z}_2$ invariants in Cu$_3$NZn are then obtained as $(\nu_0; \nu_1 \nu_2 \nu_3) = (1; 111)$, which dictate that an odd number of DLNs will pierce half the nontrivial invariant surfaces, $S_{1467}$, $S_{2457}$, and $S_{3567}$ (See Fig. 4.6).

First-principles calculations show that three distinct DLNs appear in Cu$_3$NZn, contained in the boundary planes of the BZ as shown in Fig. 4.7. For convenience,
we will refer to the DLN near the $\Gamma_i$ as $L_i$, where $i = 1, 2, 3$. The DLNs in Cu$_3$NZn form in a manner that is consistent with the topological constraint, imposed by $(\nu_0; \nu_1 \nu_2 \nu_3) = (1; 111)$. To show this, we first consider an $L_3$ that encloses $\Gamma_3$ in the BZ. As shown in Fig. 4.7, $L_3$ intersects three invariant surfaces, referred to as $S_{3567}$, $S_{0235}$, and $S_{0136}$. The $Z_2$ topological invariants $Z_2 s = (1; 111)$ dictate that $S_{3567}$ is nontrivial, and $S_{0235}$ and $S_{0136}$ are trivial, so that the nontrivial $S_{3567}$ will be pierced by an odd number of DLNs, while the trivial $S_{0136}$ and $S_{0235}$ planes will be pierced by an even (including zero) number of DLNs. It is clear from Fig. 4.7 that the trivial $S_{0235}$ and $S_{0136}$ planes are pierced by two DLNs ($L_3$ and $L_1$ for $S_{0136}$, and $L_3$ and $L_2$ for $S_{0235}$), and is thus consistent with $\xi_a \xi_b \xi_c \xi_d = 1$, where $(abcd) = (0235), (0136)$.

The nontrivial $S_{3567}$ plane also satisfies the corresponding topological constraint. To show this, we construct a $\mathcal{T}$–invariant loop $\tilde{C}_{35}$ that connects $\Gamma_3$ and $\Gamma_5$ avoiding the intersection with $L_3$ on the plane. The loop $c_{35}$ connecting $\Gamma_3$ and $\Gamma_5$ is bent down in the $-k_z$ direction, while its time–reversed partner $\tilde{c}_{35}$ is bent up in the $k_z$ direction, as shown in Fig. 4.8. From the figure, it is clear that the invariant
Figure 4.9: Band structures of Cu$_3$NX, with X=$\{V_0$, Ni, Zn$\}$. (a) Cu$_3$N. (b) Cu$_3$NNi, and (c) Cu$_3$NCu. The Dirac nodes are indicated by red circles.

surface $S_{3567}$, containing $\tilde{C}_{35}$ is pierced once by $L_3$ in its half plane, thus satisfying the topological constraint imposed by $\xi_3\xi_5\xi_6\xi_7 = -1$. Therefore, the appearance of $L_3$ satisfies the topological constraint. For the other inequivalent DLNs $L_1$ and $L_2$, the cubic symmetry of Cu$_3$NZn allows us to apply the same argument for $L_1$ and $L_2$ to conclude that all the DLNs in Cu$_3$NZn obey the topological constraints characterized by $Z_2$ topological invariants $(\nu_0; \nu_1\nu_2\nu_3) = (1; 111)$.

4.6.3 Band structures beyond Cu$_3$NZn and Cu$_3$NPd

In this section we extend our discussion of the material realization of DLN semimetals. We demonstrate that DLNs can occur in Cu$_3$N by doping a more general class of non–magnetic $3d$ and $4d$ transition metals (TMs) atoms in the $X$, $XI$, and $XII$ groups of the periodic table, and that Cu$_3$NPd$_x$ can realize DLNs in a low–doping concentration $x$ ($x < 1$). For this purpose, we first present the band structures of Cu$_3$NX, with X=$\{Ni, Cu\}$ in Fig. 4.9. These bands structures, including those of Cu$_3$NZn and Cu$_3$NPd are more or less similar, when considering the position–shift
of the Fermi energy due to the electron valence of the TM dopants. The Fermi
energy positions one band higher in the group $X_{II}$ TM–doped case, comparing to
that of the group $X$ TM–doped cases, due to two more valence electrons in the
group $X_{II}$ TMs than in the group $X$ TMs. Comparing to the band structure of
Cu$_3$N in Fig. 4.9(a), it is clear that the group $X_{II}$ TMs provide two electrons per
unit cell of Cu$_3$N, and thus move the preexisting DLNs near the Fermi energy. This
indicates that a high doping concentration $x$ should be essential in the realization
of the DLN near the Fermi energy in the group $X_{II}$–doped systems.

However, in the group $X$–doped systems, such as Cu$_3$NPd, and Cu$_3$NNi [see
Fig. 4.9(b)], these high concentrations ($x \sim 1$) are unnecessary. Under the doping
of the group $X$ TMs, the Fermi level remains in the same region as where it was
in Cu$_3$N, and instead doping drives the band–inversion. Therefore, DLNs start to
Figure 4.11: Band structures of Cu$_3$NPd with and without spin–orbit interaction. The bands in the rectangles in (a) are magnified in (b).

appear near the Fermi energy in a lower concentration regime. To demonstrate this, we calculate the band structures of Cu$_3$NPd$_x$, with $x = 0.0, 0.125, 0.25, 0.5, 0.75$ and 1.0 by varying the number of Pd atoms in a $2\times2\times2$ supercell of Cu$_3$N. The results, presented in Fig 4.10, show that the conduction and valence bands are already inverted even at $x = 0.125$, and that the degree of the band inversion, as well as the size of the DLN, increase with increasing doping concentration $x$.

Lastly, we consider the spin–orbit interaction in Cu$_3$NPd. In Fig. 4.11, we present the band structures of Cu$_3$NPd calculated with and without spin–orbit coupling (SOC). It is clear that the SOC induces a sizable gap in the DLNs up to $\sim 62$ meV along the $R$–$X$ high–symmetry line in the BZ. However, the SOC cannot completely gap out the entire DLN, as a single nodal point on the $R$–$X$ line additionally protected by a $C_4$ rotational symmetry. The states forming the nodal point have distinct eigenvalues of the rotational symmetry operation, and thus retain the degeneracy even in the presence of the SOC. This is in fact one of the mechanisms which stabilizes three–dimensional Dirac (3D) semimetals [212, 213, 244]. There-
fore one might expect the 3D Dirac semimetal phase to be present in Cu$_3$NPd. However, considering that the SOC mainly comes from the 4$d$ orbitals of Pd, and that the calculated SOC gap is estimated based on a somewhat extreme condition that Pd atoms are fully doped (one per unitcell of Cu$_3$N), it is more likely that the DLN semimetal should persist in a wide range of the Pd–doping concentration, and should be especially robust in the low–concentration regime. In order to strengthen (weaken) the SOC, one can substitute the dopants from 4$d$ TMs to 5$d$ (3$d$) TMs such as Pt (3$d$ Ni). One can even dope with magnetic TMs to explore the effect of time–reversal–symmetry–breaking in the parent DLN semimetals.
Chapter 5

Double Dirac Semimetals in Three Dimensions

5.1 Abstract

We study a class of Dirac semimetals that feature an eightfold-degenerate double Dirac point. We show that 7 of the 230 space groups can host such Dirac points and argue that they all generically display linear dispersion. We introduce an explicit tight-binding model for space groups 130 and 135. Space group 135 can host an intrinsic double Dirac semimetal with no additional states at the Fermi energy. This defines a symmetry-protected topological critical point, and we show that uniaxial compressive strain applied in different directions leads to topologically distinct
insulating phases. In addition, the double Dirac semimetal can accommodate topological line defects that bind helical modes. Connections are made to theories of strongly interacting filling-enforced semimetals, and potential materials realizations are discussed. This chapter originally appeared as an article by Benjamin J. Wieder, Youngkuk Kim, Andrew M. Rappe, and C. L. Kane in Physical Review Letters in 2016 [224].

5.2 Introduction

A striking consequence of symmetry and topology in the electronic structure of materials is the existence of protected degeneracies that guarantee semimetallic behavior. Such degeneracies occur in graphene [35] (in the absence of spin-orbit interactions) as well as at the surface of a topological insulator (TI) [83, 171]. In 2011, Wan et al. [209] pointed out that twofold degenerate Weyl points could occur in bulk 3 dimensional (3D) materials. Such Weyl points are topologically protected, though they are “symmetry prevented” in that they require broken inversion or time-reversal (T) symmetry to exist. Crystal symmetries can lead to a richer variety of nodal semimetals. Dirac semimetals [212, 213, 244], which feature fourfold degenerate Dirac points protected by crystal symmetry, occur in two varieties. Topological Dirac semimetals, such as Cd₃As₂ and Na₃Bi [24, 134, 135], exhibit Dirac points on a rotational symmetry axis due to a band inversion. Nonsymmetric Dirac semimetals, predicted in BiO₂ [244] and in BiZnSiO₄ [191], conversely
have Dirac points at high-symmetry points which are guaranteed by the underlying Space Group (SG) symmetry. Additional classes of nodal semimetals include line nodes [34, 39, 111, 112, 207, 215, 219, 220, 232, 247] in 3D and Dirac semimetals in 2D [183, 245].

In this chapter we introduce and analyze a double Dirac semimetal (DDSM) that exhibits a single eightfold degeneracy point at a Brillouin Zone (BZ) corner. We show that 7 of the 230 SGs host double Dirac points (DDPs) and argue that all of them generically have linear dispersion. For two of the SGs (130 and 135) a DDP is guaranteed whenever the band filling is an odd multiple of four, while for the remaining five SGs the presence of DDPs depends on the band ordering. We introduce an explicit tight-binding model for SGs 130 and 135 that demonstrates the DDP, and we study its low energy structure in detail. The DDSM has similar mobility and screening properties as the topological Dirac semimetal. However, the two differ fundamentally because the DDSM is symmetry tuned to a topological quantum critical point. Like the single (nonsymmorphic) Dirac semimetal, the DDSM can be gapped into a trivial or topological insulator by applying strain. In DDSMs, both phases can be achieved with compressive strain oriented along two different directions. Moreover, in the DDSM, spatially modulating the symmetry-breaking energy gap can lead to topological line defects that bind 1D helical modes. These features open new possibilities for topological band structure engineering. Materials hosting DDPs are discussed at the end of the chapter.
<table>
<thead>
<tr>
<th>Space Group</th>
<th>Reps at K</th>
<th>Vector Reps</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P4/ncc$</td>
<td>$D_4^h$</td>
<td>$\Gamma_5^{12}(8)$</td>
</tr>
<tr>
<td>$P4_2/mnc$</td>
<td>$D_{13}^h$</td>
<td>$\Gamma_5^{12}(8)$</td>
</tr>
<tr>
<td>$P4_3m$</td>
<td>$T_3^4$</td>
<td>$\Gamma_6 \oplus \Gamma_7(4), \Gamma_8^{12}(8)$</td>
</tr>
<tr>
<td>$P4_3d$</td>
<td>$T_3^5$</td>
<td>$\Gamma_6 \oplus \Gamma_7(4), \Gamma_8^{12}(8)$</td>
</tr>
<tr>
<td>$Pn3n$</td>
<td>$O_2^6$</td>
<td>$\Gamma_6(4), \Gamma_6 \oplus \Gamma_7(8)$</td>
</tr>
<tr>
<td>$Pm3n$</td>
<td>$O_3^6$</td>
<td>$\Gamma_6(4), \Gamma_6 \oplus \Gamma_7(8)$</td>
</tr>
<tr>
<td>$Ia3d$</td>
<td>$O_5^{10}$</td>
<td>$\Gamma_5(4), \Gamma_6 \oplus \Gamma_7(8)$</td>
</tr>
</tbody>
</table>

Table 5.1: Space groups that host DDPs. SGs are indicated in International notation as well as in Schönflies notation, which indicates the crystal system and point group. The momenta $K$ are listed with symmetry labels for the 8DIRs, as well as for some 4DIRs. The final column indicates the $T$-invariant vector representations of the point group contained in the tensor product $\Gamma^* \otimes \Gamma$ of the 8DIR at $K$, indicating that in each case a linear dispersion is generic.

### 5.3 8-Dimensional Irreducible Representations

The existence of symmetry-protected degeneracies at a point $K$ in the BZ can be ascertained by determining the dimension of the appropriate double-valued projective representations of the little group of $K$. This information has been tabulated for all 230 SGs [26]. Table 5.1 lists all of the SGs with symmetry points that host Four-Dimensional Irreducible Representations (4DIR) that are also doubled by $T$ symmetry[139].

SGs 130 and 135 have the distinguishing feature that there is only a single 8DIR at the $A$ point. Therefore groups of 8 bands “stick together”, implying an insulator is only possible when the band filling is a multiple of 8. Interestingly, Watanabe et al. [216](WPVZ) recently introduced a bound on the minimal filling for an insulator that applies to strongly-interacting systems. The WPVZ bound for SG 130 is 8, in agreement with the band theory analysis, while for SG 135 the WPVZ bound of 4 disagrees with band theory [216]. Below we show that for SG 130, but not for SG
135, additional single Dirac points are present when the filling is an odd multiple
of 4. Since the energy of the single and DDPs will differ, SG 130 will generically
host a semimetal with electron and hole pockets. In contrast, in SG 135 the DDP
is the only required degeneracy, so SG 135 can host an intrinsic DDSM. The fact
that the symmetry-guaranteed DDP is not covered by the WPVZ bound poses the
interesting question of whether strong interactions can open a symmetry-preserving
gap in SG 135.

For the remaining 5 SGs in Table 5.1 there are 4DIRs in addition to the 8DIRs
at $K$. Therefore, the presence of DDPs at the Fermi level depends on the band
ordering, as it does in group IV semiconductors where band inversion in grey tin
leads to a fourfold degeneracy at $E_F$ [75] with quadratic dispersion. To determine
whether the dispersion at the DDPs is linear we check whether the $\mathcal{T}$-odd vector
representation(s) are contained in the tensor product $\Gamma \otimes \Gamma^*$ of the 8DIR at $K$ [244].
This is found by computing the character of the symmetric Kronecker square [26]
of $\Gamma$ and using the orthogonality of characters to project onto the vector representa-
tion. This analysis, which agrees with the specific example worked out below,
predicts the multiple vector representations listed in Table 5.1. Therefore in all
cases the dispersion near $K$ will generically be linear. The DDP is anisotropic for
the tetragonal structures 130 and 135, while for the remaining cubic structures it
is isotropic.
We now introduce an explicit tight-binding model for SGs 130 and 135. These SGs share the same tetragonal structure and are characterized by the symmetry generators in Table 5.2. We introduce a unit cell (Fig. 5.1(a)), with 4 sublattices indexed by $(\tau^z, \mu^z) = (\pm 1, \pm 1)$ associated with basis vectors $d = \frac{1}{2}[(1 - \tau^z)(1 \frac{1}{2} 0) + (1 - \mu^z)(00 \frac{1}{2})]$. This can be viewed as a distortion of a parent Bravais lattice [245] in which the 4 sublattices are related by pure translations. Nearest neighbor hopping on this parent lattice is described by

$$\mathcal{H}_0(\mathbf{k}) = t_{xy} \tau^x \cos \frac{k_x}{2} \cos \frac{k_y}{2} + t_z \mu^z \cos \frac{k_z}{2},$$  \hspace{1cm} (5.4.1)
where we choose a gauge in which the state associated with sublattice \((\tau^z, \mu^z)\) has phase \(\exp i k \cdot d\), so

\[
\mathcal{H}(k + \mathbf{G}) = e^{-i \mathbf{G} \cdot \mathbf{d}(\tau^z, \mu^z)} \mathcal{H}(k) e^{i \mathbf{G} \cdot \mathbf{d}(\tau^z, \mu^z)}. \tag{5.4.2}
\]

SGs 130 and 135 involve lowering the translational symmetry while keeping different nonsymmorphic glide and screw symmetries. The symmetry generators are represented by operators on the 8-dimensional spin and sublattice space \(D(\{g|t\})\) listed in Table 5.2. In addition, \(\mathcal{T}\) symmetry is represented by \(\mathcal{T} = i \sigma^y \mathbf{K}\). Symmetry-lowering perturbations \(\mathcal{H} = \mathcal{H}_0 + V\) must satisfy

\[
V(gk) = D(\{g|t\}) V(k) D(\{g|t\}), \tag{5.4.3}
\]

\[
V(-k) = \Theta V(k) \Theta^{-1}. \tag{5.4.4}
\]

It is straightforward to enumerate the allowed terms for each SG. In general, there are 28 terms consistent with inversion and \(\mathcal{T}\). Eqs. 5.4.2-5.4.4 determine the \(k\) dependence of each term. Here, in order to faithfully characterize the degeneracy pattern of the band structures we consider a simplified model with a subset of crystal field, hopping and spin orbit terms that respect (5.4.4) and are sufficient.
to lift all nonessential degeneracies. These qualitative features are reflected in the specific materials band structures discussed in the supplementary materials.

\[ V_{130} = \lambda_1 \tau^z \mu^y \cos \frac{k_x}{2} + \lambda_2 \tau^z (\sigma^x \sin k_y - \sigma^y \sin k_x) \]

\[ + \lambda_3 \tau^z \mu^z (\sigma^x \sin \frac{k_x}{2} \cos \frac{k_y}{2} + \sigma^y \cos \frac{k_x}{2} \sin \frac{k_y}{2}), \quad (5.4.5) \]

and

\[ V_{135} = t'_1 \mu_z (\cos k_x - \cos k_y) + t'_2 \tau^y \mu^y \sin \frac{k_x}{2} \sin \frac{k_y}{2} \cos \frac{k_x}{2} \]

\[ + \lambda'_1 \tau^z \mu^x (\sigma^x \sin \frac{k_x}{2} \cos \frac{k_y}{2} + \sigma^y \cos \frac{k_x}{2} \cos \frac{k_y}{2} \sin \frac{k_x}{2}) \sin \frac{k_x}{2} \]

\[ + \lambda'_2 \tau^x \mu^y (\sigma^x \cos \frac{k_x}{2} \sin \frac{k_y}{2} + \sigma^y \sin \frac{k_x}{2} \cos \frac{k_y}{2} \sin \frac{k_x}{2}) \sin \frac{k_x}{2} \]

\[ + \lambda'_3 \tau^y \mu^z \sigma^z \cos \frac{k_x}{2} \cos \frac{k_y}{2} (\cos k_x - \cos k_y). \quad (5.4.6) \]

Fig. 5.1(c,d) show energy bands associated with these models. Each band is at least doubly degenerate. Both cases feature a DDP at \( A \) with linear dispersion in all directions. SG 130 features an additional fourfold crossing along the line \( Z-R \). This crossing is protected by \( T \), inversion and the \( C_{2x} \) screw, whose axis is displaced from the center of inversion. This guarantees that the Kramers-degenerate pairs of states on this line share the same eigenvalue of the \( C_{2x} \) screw, allowing pairs with different eigenvalues to cross. A similar crossing occurred in the Dirac ring found in Refs. 34, 111 and was locally characterized in Ref. 56. In fact, this crossing is guaranteed by symmetry, since it is not possible to eliminate it by reordering the
bands at $Z$ or at $R$. This pattern of degeneracies guarantees that groups of 8 bands stick together, independent of the DDP at $A$, and appears to be correlated with the WPVZ bound.

Since the additional Dirac points need not be at the same energy as the DDP, SG 130 will generically be a semimetal with electron and hole pockets. In contrast, SG 135 has no additional Dirac points, so it can host an intrinsic DDSM. However, we find that for $\lambda'_2 > \lambda'_1$ there are additional single Dirac points along the lines $A-Z$. These arise due to a “velocity inversion” transition at $\lambda'_2 = \lambda'_1$, which we analyze below. A similar velocity inversion occurs in 130 for $\lambda_3 > 2\lambda_2$.

We now focus on SG 135 and consider the low energy structure near the DDP. There are no symmetry-respecting terms at $A$ that lift the degeneracy. To determine the terms linear in $k$ we identify the $T$-odd operators transforming in the vector representations of the point group $D_{4h}$. Using (5.4.2-5.4.4), the representations of the symmetry operations at $A$ are $d_A(\{C_4|00\}) = \tau^z\mu^x \exp i\pi \sigma^z/4$, $d_A(\{C_2|0\}) = \tau^y\mu^z \sigma^x$ and $d_A(\{I|000\}) = \mu^z$. Also, $T_A = i\mu^z \sigma^y K$. We find 4 (3) terms with $E_u$ ($A_{2u}$) symmetry, in agreement with the general analysis of Table 5.1. The $k \cdot p$ Hamiltonian at $A$ is

$$H_A = (u_0\tau^x \mu^y \sigma^z + u_1\tau^y \mu^x \sigma^y + u_2\mu^y \sigma^y + u_3\tau^z \mu^y \sigma^z)k_x$$

$$+ (u_0\tau^x \mu^y \sigma^y + u_1\tau^y \mu^x \sigma^x + u_2\mu^y \sigma^x - u_3\tau^z \mu^y \sigma^y)k_y$$

$$+ (v_1\mu^x + v_2\tau^y \mu^y + v_3\tau^x \mu^y \sigma^z)k_z.$$  (5.4.7)
This leads to dispersion

\[
E_\pm^2(k) = (|u|^2 + u_0^2)(k_x^2 + k_y^2) + |v|^2k_z^2 \\
\pm 2\sqrt{4k_x^2k_y^2}|u|^2u_0^2 + (k_x^2 + k_y^2)k_z^2(u \cdot v)^2, \tag{5.4.8}
\]

where \(u = (u_1, u_2, u_3)\) and \(v = (v_1, v_2, v_3)\). When \(|u_0| = |u|\), one of the branches vanishes on the line \(k_x = k_y, k_z = 0\), identifying the velocity inversion transition along \(A-Z\) discussed above. From the tight-binding model, we have \(u = (\lambda_1', 0, 0)\), \(u_0 = \lambda_2\), so we identify \(|u_0| < |u|\) with the intrinsic DDSM phase with no additional degeneracies.

Lowering the symmetry by external perturbations, such as strain, provides a powerful tool for engineering gapped topological phases\[29, 61\] We therefore consider the long-wavelength symmetry-breaking perturbations that open energy gaps and identify the resulting phases that arise. General symmetry-breaking perturbations are classified by their symmetries under the \(D_{4h}\) point group, which can be

<table>
<thead>
<tr>
<th>(A_{1g})</th>
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<th>Double Dirac SM</th>
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determined from \( d_A(\{g|\mathbf{t}\}) \), as above. The possible \( \mathcal{T} \)-invariant perturbations at \( A \) are listed in Table 5.3. There are many terms, and their effects depend on the form of the velocity terms. In order to organize the behavior, we first fix the velocity terms and examine the terms that can open a gap in the spectrum. We find that there are precisely four mass terms that arise due to perturbations with specific symmetries. The Hamiltonian has the form

\[
\mathcal{H} = u_2 \mu^y (\sigma^y k_x + \sigma^x k_y) + v_1 \mu^z k_z + m_{A_{2g}} \tau^x \mu^z + m_{B_{2g}} \tau^z \mu^z + m_{B_{1g}} \mu^z + m_{A_{1u}} \tau^y \mu^y \sigma^z. \tag{5.4.9}
\]

The four mass terms are the unique terms from Table 5.3 that anticommute with all three of the velocity terms and open a gap. They fall into two groups. \( \mathbf{m}_1 = (m_{A_{2g}}, m_{B_{2g}}) \) and \( \mathbf{m}_2 = (m_{B_{1g}}, m_{A_{1u}}) \) anticommute among themselves but commute with each other, leading to an energy gap \( E_{\text{gap}} = 2|m| \) with \( m = |\mathbf{m}_1| - |\mathbf{m}_2| \). There are two phases distinguished by \( \text{sgn}(m) = +1(-1) \). Using parity eigenvalues \([61, 65]\), we identify them as a \([0; 110]\) weak TI (\([1; 001]\) strong TI). While these indices depend on the details of the band structure away from the DDP, the difference between the phases is robust. To visualize the phases, Fig. 5.2(a) shows a phase diagram for \( m_{A_{1u}} = 0 \). In this 3D space, the STI (WTI) are inside (outside) a cone. In the more general 4D phase diagram, the WTI and STI phases appear symmetrically.

Different combinations of velocity terms lead to different choices for the anticom-
mutation mass terms. However, for any combination of velocity terms in (5.4.7), it can be exhaustively checked that there is one anticommuting term with each of the symmetries in Eq. 5.4.9. Therefore, a generic perturbation with a given symmetry induces the corresponding mass term and opens a gap. The general structure of Fig. 5.2(a) remains, except that when the inversion-symmetry-breaking term $m_{A_{1u}}$ is present the boundary between the STI and WTI phases broadens to include a Weyl semimetal phase [154].

The dependence of the topological state on $m_{B_{1g}}$ and $m_{B_{2g}}$ provides a mechanism for controlling topological states using strain. As indicated in Fig.5.2(b,c), uniaxial strain along the $x$ or $y$ directions induces a perturbation with a combination of $A_{1g}$ and $B_{1g}$ symmetry, while uniaxial strain along the diagonal $x \pm y$ directions has $A_{1g}$ and $B_{2g}$ symmetry. Therefore these two kinds of compressive strain lead to topologically distinct insulators.
5.5 Discussion

DDPs can also be differentiated from single Dirac semimetals by the existence of two distinct anticommuting mass terms that lead to the same topological phase. For a single Dirac semimetal with $4 \times 4$ Dirac matrices, the general structure of Clifford algebras predicts that there is only a single $\mathcal{T}$-invariant mass term that anticommutes with the three $\mathcal{T}$-odd anticommuting velocity terms. For $8 \times 8$ Dirac matrices there are two anticommuting $\mathcal{T}$-invariant mass terms. This means that the space of gapped states has a nontrivial first homotopy group, indicated by the dashed circle in Fig. 5.2(a), allowing topologically nontrivial line defects (Fig. 5.2(d)). Line defects in a 3D insulator in class AII have a $Z_2$ topological invariant characterizing the $3 + 1$D $\mathcal{H}(\mathbf{k}, \theta)$ [200]. When nontrivial, this guarantees that a 1D helical mode is bound to the line, similar to the helical mode bound to a lattice dislocation in a weak TI [174]. Without a lattice dislocation, this $Z_2$ invariant is inaccessible in a 4 band system because it derives via dimensional reduction [170] from a third Chern number in $3 + 1 + 2$D, which requires at least 8 bands. To establish that a line defect binds a 1D helical mode, we follow the analysis of Ref. 200, and consider a simple model with $m_{B_{2g}} = ax$, $m_{A_{2g}} = ay$ and $u_1 = v_2 = v$. $\mathcal{H}^2$ in (5.4.9) then has the form of a harmonic oscillator, and there is a single pair of modes with $E = \pm v k_z$ localized near $x = y = 0$.

We finally briefly consider perturbations in Table 5.3 with the remaining symmetries, which lead to Weyl or Dirac semimetals. The $E_g$ perturbations lead to either
Dirac points or a Dirac ring, with fourfold-degenerate crossings. The inversion breaking-perturbations generally lead to a Weyl semimetal with twofold crossings, except for $A_{2u}$, where the remaining $C_{2z}$ and glide mirror symmetries guarantee doubly-degenerate states for $k_x = k_y = \pi$ with the same $C_{2z}$ eigenvalue. This allows degenerate bands to cross along $A-M$, protecting a Dirac point even though inversion is violated.

Encouragingly, the DDP appears to be feasible in known materials. For example, a ternary bismuth aurate, $\text{Bi}_2\text{AuO}_5$ in SG 130, which has been synthesized in a single crystal [69], hosts a DDP at $A$ close to the Fermi level, with additional four-fold degeneracies appearing on $Z-R$ (Fig. 5.3). As for materials in SG 135, the Materials Project [99] shows that a class of oxide materials isostructural with $\text{Pb}_3\text{O}_4$ [67], including $\text{Sn(PbO}_2)_2$, $\text{Pb}_3\text{O}_4$, and $\text{Mg(PbO}_2)_2$, host the DDPs in the valence energy regime. Although they are semiconductors with electron filling 8, their atomic structure allows for a potential route towards a material design that shifts

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1See Supplemental Material, which includes Refs. [72, 85, 167, 173, 175], for the band structures.
the Dirac point near the Fermi level. The number of atoms per each species in a unit cell is 4 \((\text{mod } 8)\) and thus allows for filling 4 when suitably substituting atoms with an odd number of valence electrons. In SG 223, GaMo$_3$ [25] hosts a DDP. There is reason for optimism that with appropriate band structure engineering, an intrinsic DDSM can be realized.

5.6 Chapter Acknowledgments

We thank Eugene Mele and Steve Young for helpful discussions. This work was supported by NSF grant DMR 1120901 and a Simons Investigator grant to CLK from the Simons Foundation. AMR acknowledges the support of the DOE, under grant DE-FG02-07ER46431.

5.7 Supplemental Material

5.7.1 Computational Methods

We perform \textit{ab initio} calculations based on Density Functional Theory (DFT) to find the band structures of Bi$_2$AuO$_5$, Sn(PbO$_2$)$_2$, Pb$_3$O$_4$, and GaMo$_3$. We use the Perdew–Burke–Ernzerhof–type generalized gradient approximation [167] as found in the \textsc{Quantum Espresso} package [72]. Norm–conserving, optimized, designed non-local pseudopotentials are generated using the \textsc{Opium} package [173, 175]. An energy
cutoff of 680 eV is used for the plane–wave basis. A fully-relativistic non–collinear scheme is employed to describe spin-orbit interaction. The atomic structures are obtained from the inorganic crystal structure database (ICSD) database [85].

5.7.2 Double Dirac Points in Real Materials

Here we present our DFT band structures of real materials that host the double Dirac point. We have searched the MATERIALS PROJECT [99] to find stable crystals in the space groups 130, 135, 218, 220, 222, 223, and 230, resulting in the following set of candidate materials.

5.7.2.1 Bi$_2$AuO$_5$ in space group 130

The energy band structure of Bi$_2$AuO$_5$ in space group 130 is shown in Fig. 5.4. The band structure is drawn along the high–symmetry lines of the tetragonal BZ, shown in the upper panel. The Fermi level is set to 0 eV. The double Dirac point (indicated by a blue circle) appears at A in good agreement with the results of the four-site tight-binding model. There is an additional Dirac point in R-Z, guaranteed by symmetry, which is magnified in the upper inset. We expect that Bi$_2$AuO$_5$, which has been synthesized in a single-crystal phase [69], should realize a double Dirac semimetal.
Figure 5.4: Electronic band structure along high–symmetry lines in Bi$_2$AuO$_5$ in space group 130.

5.7.2.2 Sn(PbO$_2$)$_2$ in space group 135

In Fig. 5.5, the electronic energy band structure of Sn(PbO$_2$)$_2$ in space group 135 is presented. The Fermi level is set to 0 eV and the valence bands are plotted along high–symmetry lines of the tetragonal BZ. The double Dirac point is enclosed by a blue-colored circle. The number of Sn, Pb, and O atoms in the unit cell are 4, 8, and 16, respectively, and the number of valence electrons of Sn, Pb, and O are 14, 14, and 6, respectively, and thus the total number of valence electrons is 72. Although Sn(PbO$_2$)$_2$ is an insulator with filling zero (mod 8), a double Dirac point appears in the valence band at 0.54 eV below the Fermi level. The atomic structure of Sn(PbO$_2$)$_2$ [67] allows for the possibility of utilizing material design to shift the Fermi energy closer to the double Dirac point. For example, when Sn is
substituted with In or Sb, which have one less or one more valence electron than Sn, respectively, the electron filling can change from zero to four (mod 8), possibly hosting the double Dirac point close to the Fermi energy.

### 5.7.2.3 Pb$_3$O$_4$ in space group 135

Figure 5.6 shows the band structure of Pb$_3$O$_4$ in space group 135. Pb$_3$O$_4$ is isostructural with Sn(PbO$_2$)$_2$ with Sn being substituted by Pb. The band structure also
Figure 5.7: Electronic band structure of GaMo$_3$ in space group 223.

resembles that of Sn(PbO$_2$)$_2$. A double Dirac point resides at $A$ in the valence band region near $E = -0.57$ eV.

5.7.2.4 GaMo$_3$ in space group 223

The electronic energy bands of GaMo$_3$ [25] are drawn in Fig. 5.7 along the high-symmetry lines of the cubic BZ, depicted in the inset. The position of the double Dirac point is indicated by a blue-colored circle.
Chapter 6

Minimal Insulating Filling and the Layer Groups

6.1 Abstract

Recent interest in point and line node semimetals has led to the proposal and discovery of these phenomena in numerous systems. Frequently, though, these nodal systems are described in terms of individual properties reliant on specific space group intricacies or band-tuning conditions. Restricting ourselves to cases with strong spin-orbit interaction, we develop a general framework which captures existing systems and predicts new examples of nodal materials. In many previously proposed systems, the three-dimensional nature of the space group has obscured
key generalities. Therefore, we show how within our framework one can predict and characterize a diverse set of nodal phenomena even in two-dimensional systems constructed of three-dimensional sites, known as the “Layer Groups”. Expanding on an existing discussion by Watanabe, Po, Vishwanath, and Zaletel of the relationship between minimal insulating filling, nonsymmorphic symmetries, and compact flat manifolds, we characterize the allowed semimetallic structures in the layer groups and draw connections to related three-dimensional systems. This chapter originally appeared as an article by Benjamin J. Wieder and C. L. Kane in Physical Review B in 2016 [221].

6.2 Introduction

Nodal semimetals are systems of arbitrary dimensionality for which the valence and conduction bands meet and form nodes in a limited set of places in the Brillouin zone. The existence of nodal points at the Fermi energy has implications for bulk transport, surface physics, and is even related to topology [2, 65, 66, 106, 156, 159, 189]. Since the discovery of nodal points with linear dispersion in single-sheet graphene [35, 208], there has been great effort to locate and characterize similar band-touching nodes in other systems. Rich nodal physics can also be found in graphene bilayers, however these systems have quadratically-dispersing nodes, and thus differing transport properties and gapped phases [35, 144, 146, 161, 163, 223, 254]. Therefore, this search for graphene-like physics can be considered
more specifically a search for systems with *linearly-dispersing* nodal points at the Fermi energy.

Extending this search to three dimensions, there are generically two realizations of this nodal physics: point nodes and nodal lines. Bands can meet at nodes with linear dispersion in three directions and form Dirac or Weyl points, with four- and two-fold nodal degeneracies respectively [24, 32, 38, 55, 86, 95, 122, 135, 191, 209, 235, 236, 240, 244], or in unusual three-, six-, and eight-fold degeneracies [27, 224]. Bands can also meet and form line nodes, or lines along which there is no dispersion in one direction and linear dispersion in the remaining two directions [21, 34, 40, 41, 73, 112, 207, 219, 220, 232, 247, 251].

Each of these examples of nodal phenomena owes its protection to some combination of topology and exact crystalline symmetries. However, many of them have been described in terms of individual properties, such as topological invariants and symmetry eigenvalues. In this chapter, we seek to provide a more generalized consideration of those nodal systems protected by crystalline symmetries, as well as a means to sort and classify them.

### 6.2.1 The Two Flavors of Semimetals

As a starting point for sorting these various nodal materials, one could ask whether or not any of their nodal features can be eliminated to open a gap. Consider
the ability to remove point nodes pairwise, or to shrink and gap line nodes at a point, while still preserving a system’s crystalline symmetries. The Dirac points in Cd$_3$As$_2$ and Na$_3$Bi, as well as the line nodes proposed in Cu$_3$N and observed in Ca$_3$P$_2$ [24, 112, 135, 232, 247], obey this property, whereas the proposed Dirac points in BiO$_2$ and the Dirac line nodes in SrIrO$_3$ do not [34, 244]. We can designate this first category of nodal systems as band-inversion semimetals. The nodes in these systems are optional features of the space group; they are certainly locally permitted by crystalline symmetries, or topology in the case of Dirac line nodes under weak spin-orbit interaction, but they are otherwise globally extraneous. Conversely, the nodes in BiO$_2$ and SrIrO$_3$ are part of groupings of 4 and 8 bands, respectively. All of the bands in these systems appear at a minimum in groupings of these numbers, and the existence of nodal features at the Fermi energy appears to be guaranteed by the electron filling. We therefore designate these as essential semimetals, or systems with nodes which are pinned into existence by additional space-group-specific symmetries.

This relationship between essential nodal features and filling is, as discussed in this chapter, the single-particle manifestation of the concept of “minimal insulating filling.” Watanabe, Po, Vishwanath, and Zaletel (WPVZ) realized that for 220 of the 230 space groups, a discussion of related flat compact manifolds allows one to exclude the existence of an insulating state at fillings specific to each space group [216]. Note that this criterion only addresses the allowed existence of a consistent band gap for systems in which all bands are either fully occupied or
unoccupied. It does not exclude cases where the dispersion is large and the Fermi energy cuts through electron and hole pockets. Nevertheless, for the purposes of this chapter, we will still refer to such indirect gap materials as insulators, as many of the analysis methods for such systems, such as polarization and topological invariant calculations, only require the ability to find well-separated band groupings.

In this chapter, we designate the integer fillings at which WPVZ deduced an allowed insulating state as the “WPVZ bound.” In the limit that interactions are weak and bands are well-defined, we observe that the same combinations of crystalline symmetries which define the WPVZ bound also conspire to guarantee essential groupings of bands. Furthermore, in cases where local topological features might be removed to open a gap, such as the combination of two Weyl points with opposite Chern numbers [209], this bound provides an obstruction to that process. For example, if two Weyl points are required to exist by minimal insulating filling, they cannot be gapped out while preserving all crystalline symmetries, even if they have opposite Chern numbers, as the bands which comprise them cannot be separated without lowering the system symmetry and changing the space-group-specific filling constraints.

In practice, the determination of this bound, as well as the accompanying analysis of crystalline symmetry algebra, can become difficult in three dimensions. Noting that Young and Kane also predicted essential semimetallic features in two-dimensions [245], we therefore propose a consideration of the WPVZ bound and the
allowed nodal features in two dimensions. Furthermore, to restrict our discussion to the role of crystalline symmetries, we require strong spin-orbit interaction, such that locally-protected topological features, such as the Dirac points in graphene, are disallowed. In this chapter, we observe that, considering the full set of 80 two-dimensional systems known as the “layer groups” [87], nontrivial WPVZ bounds can be achieved and rich nodal semimetallic phenomena can be both created in band-inversion semimetals and required in essential semimetals. Some of these phenomena are protected by the same mechanisms as are their three-dimensional cousins that occur in such materials as BiO$_2$ and SrIrO$_3$. Furthermore, we show how this analysis predicts previously uncharacterized nodal phenomena in two- and three-dimensions, such as band-inversion Dirac points protected by an inversion-center offset and an essential 8-band “cat’s cradle” Weyl fermion feature.

6.2.2 Contents of this Chapter

This chapter is structured as follows. First, in 6.3 we use a discussion of compact flat manifolds to rederive the WPVZ bound in first purely two-dimensional systems (wallpaper groups) and then in two-dimensional systems embedded in three dimensions (layer groups). Following that, we provide in 6.4 a breakdown of the eigenvalue structure of band groupings as it relates to spatial symmetries and inversion centers. Finally, in 6.5 we combine both descriptions to produce criteria for predicting semimetallic features and apply them to a set of related simple models.
Figure 6.1: The 3 compact manifolds which can be achieved by twisting the coordinate-axis-direction boundary conditions for a strictly two-dimensional system that is periodic in both in-plane directions. The local designations of the perpendicular direction are indicated by the arrows, a notation known as the “fundamental polygon.” Of the possible manifolds, the 2-torus (a) and the Klein bottle (b) are flat, but the real projective plane \((RP^2)\) (c) is not. Flatness can be evaluated by testing for the existence of fixed or special points by drawing a circle centered on the boundary and comparing its circumference to that of a circle drawn on the interior. Staring at the bottom left corner, the dashed line indicates the boundary of a circle of radius \(r\). For the 2-torus and the Klein bottle, this boundary explores all four corners, resulting in a circumference of \(2\pi r\), matching the value on the interior. However, for \(RP^2\), this boundary only additionally explores the top right corner before returning, resulting in a reduced circumference of just \(\pi r\), and indicating that the two bottom corners are special points, distinct from the interior and from each other, and therefore that \(RP^2\) is not uniform. The bold numbers indicate the number of times that each pattern would have to be repeated to create a supercell with the same boundary conditions as the initial 2-torus. Pictorial guides to forming such supercells can be found in Appendix 6.8.1.

characteristic of both band-inversion and essential nodal semimetallic features in two-dimensional crystals with strong spin-orbit interaction.

### 6.3 Platycosms and Minimal Insulating Filling

To begin, we relate the idea of minimal insulating filling to the compatibility between a given two-dimensional group and a set of flat compact manifolds. Recent work by Watanabe, Po, Vishwanath, and Zaletel (WPVZ) has revived interest in
this relationship between the space groups and three-dimensional manifolds [216].

To introduce this topic, we begin with a review of familiar manifolds in two dimensions. We then extend this discussion to encompass layered three-dimensional systems. Finally, we conclude this section with a review of the WPVZ arguments for minimal insulating filling and how those arguments relate to the sets of compact flat manifolds in two and three dimensions.

This discussion is intended as an introduction to topics in topology and group theory such as compact manifolds and group modding procedures. At the level of this chapter, we loosely equate such concepts as flatness, uniformity, and the absence of fixed points. For a more formal treatment of this material, we recommend that one consult Conway and Rossetti [89].

6.3.1 Compact Flat Manifolds in Two and Three Dimensions

For a 2D system periodic in one of the in-plane directions, say a piece of paper wrapped onto itself, there are two ways to assign boundary conditions. Linking the two opposite sides without any twists produces a cylinder, and twisting the paper once produces the familiar Möbius strip. We can also consider a 2D object with periodicity in both of the in-plane directions. Visually, one can assign boundary conditions for such an object by considering the orientation of arrows on the fundamental polygon (Fig. 6.1).
The three distinct combinations of arrow assignments for a two-dimensional system with two periodic directions give a 2-torus, a Klein bottle, and the real projective plane ($RP^2$). Keeping the arrow assignments consistent relative to the left-hand side of the polygon, one could produce a pattern like the one on a 2-Torus (Fig. 6.1(a)) by linking together \textit{twice} a Klein bottle (Fig. 6.1(b)) or \textit{four times} $RP^2$ (Fig. 6.1(c)). The creation of such a supercell from the various manifolds is visually depicted in Appendix 6.8.1.

These manifolds can accommodate the set of truly two-dimensional systems, that is, systems comprised of two-dimensional objects embedded in a two-dimensional space. Some of these manifolds permit the embedding of a subset of systems known as the \textit{Wallpaper Groups} [44]. When considered in three dimensions, the wallpaper groups consist of the 17 unique combinations of symmetries which could describe the two-dimensional boundary of a three-dimensional object. They are therefore characterized only by symmetry operations which preserve the interior and exterior of such a boundary, namely mirror and glide lines in the plane and rotations of the surface about its normal vector. For this reason, the operation of an arrow flip could also be considered the modding out of a glide mirror, as a site on the left side of a \textit{flipped} boundary is related to a site on the right side by a glide mirror operation.

Modding out a single glide produces the Klein bottle (Fig. 6.1(b)): a two-dimensional manifold that has just one surface (also sometimes called nonorientable
as its surface does not preserve the handedness of a coordinate axis which traverses it) [89]. This object is compact, as it was constructed periodically, and but it is also flat. Modding out an additional glide produces the one-sided real projective plane ($RP^2$) (Fig. 6.1(c)), which unlike the 2-torus and the Klein bottle has fixed points, and is therefore not flat and uniform.

One can test for these fixed or special points in two dimensions by considering the circumference of a circle of radius $r$ centered throughout the manifold. In the center of all three two-dimensional manifolds, this circle has circumference $2\pi r$. The only possible deviations from this value can occur at the boundaries of the manifolds, as depicted by the dashed lines in Figure 6.1. For the 2-torus and the Klein bottle, the boundary of a circle of radius $r$ centered at the bottom left corner still explores all three other corners before returning, resulting in a circumference of $2\pi r$, a value that matches circles on the interior. However, for $RP^2$, the boundary returns to itself after only reaching the top right corner, giving a circumference of just $\pi r$, and indicating that the two bottom corners are special points, different from each other and from the interior.

A key restriction of WPVZ’s argument is that any manifold for consideration must allow the uniform embedding of a crystal lattice such that the Bloch wave functions are periodic plane waves [216]. The special corners in $RP^2$ violate this uniformity, and therefore modding out onto it is disallowed. We therefore conclude that the wallpaper groups can only be uniformly embedded on the 2-torus and on the
More formally, we can consider this restriction to fixed-point-free manifolds in terms of group theory. WPVZ take advantage of work by Bieberbach that established that a collection of 10 space groups are fixed-point free. These space groups each have only one nonsymmorphic symmetry, or have a very special combination of two perpendicular nonsymmorphic symmetries such that no fixed points are introduced. We note that for just one of these 10 space groups, there is a corresponding wallpaper group. This wallpaper group, \( pg \) (space group 7 \( Pb11 \)), is characterized just by a single glide symmetry. The process of modding out a glide and flipping an arrow on the fundamental polygon is more formally asking whether or not \( pg \) is a subgroup of that wallpaper group, such that it can be modded out. As \( pg \) only contains one glide, modding by it results in a placement onto the Klein bottle, and as none of the remaining nonsymmorphic wallpaper groups correspond to fixed-point-free space groups when stacked in three dimensions, the Klein bottle is the only manifold besides the 2-Torus which is compatible with the embedding of a purely two-dimensional crystal lattice. Finally, as only nonsymmorphic operations can provide a coordinate-arrow twist of the fundamental polygon, and as all of the nonsymmorphic wallpaper groups describe rectangular lattices, we therefore find that all possible restrictions on the uniform embeddings of 2D lattices can be obtained by considering whether or not axis boundary condition flips on the fundamental polygon introduce fixed points.
Figure 6.2: The compact, flat manifolds which can be achieved in three-dimensional, layered systems. The notation used is a modification of the fundamental polygon from Figure 6.1 by the additional local assignment of the stacking direction as indicated by the $\oplus$ and $\ominus$ signs. Unlike in the strictly two-dimensional wallpaper systems, the modding out of a two-fold screw is also allowed and leads to a new manifold which doesn’t decompose into $S^1$ multiplied by a wallpaper manifold. Modding out a screw preserves the interior and exterior surfaces leading to the dicosm (b). Modding out a glide reduces the system to being one-sided and leads to the 1st amphicosm (c). In these layered systems, unlike in the 2D wallpaper cases, a particular combination of two perpendicular nonsymmorphic operations can be modded out without introducing fixed points, leading to a new flat manifold: the 1st amphidicosm (d). The bold numbers indicate the number of times that each pattern would have to be repeated to create a supercell with the same boundary conditions as the initial 3-torus (a). The procedure for forming such supercells is explained with visuals in Appendix 6.8.1.
In three-dimensions, this argument can be extended, though unfortunately in
genral there is no neat analogue to the fundamental polygon to describe the equiva-
ent operations of modding out glide mirrors or screws. The 10 resultant three-
dimensional flat manifolds are known as the platycosms. Descriptions of them, as
well as, where possible, connections to more familiar manifolds, are detailed in plain
language in Ref. 89.

However, for 80 realizations of 70 three-dimensional space groups, crystals can
be decomposed into two-dimensional sheets, only related to the next layer by lattice
periodicity in the stacking direction. For these layered systems, symmetry-enforced
physics is entirely determined by the symmetries of a two-dimensional single layer,
and therefore even though they are three-dimensional systems, many of their prop-
erties can be determined by confining analysis to the two-dimensional subsystem
of a single layer. These single-layer systems, comprised of two-dimensional objects
embedded in three dimensions, are a subset of “subperiodic groups” known as the
Layer Groups [87].

For these layer group systems, placement onto a platycosm can be visually repre-
sented by modifying the fundamental polygon to include a local specification of the
̃ direction (stacking direction) (Fig. 6.2). For these systems the modding out of a
two-fold screw is now also permitted in addition to the glide mirror mod, with the
screw mod taking one to the two-sided dicosm (Fig. 6.2(b)) and the glide mod tak-
ing one to the one-sided 1st amphicosm (Fig. 6.2(c)) (which can also be expressed
as *klein bottle* × $S^1$) [89, 216]. Remarkably, the modding out of a glide which flips
the $\hat{z}$ direction as well as a perpendicular screw results in a manifold which, unlike $RP^2$ in the fully-two-dimensional wallpaper systems, is flat. This manifold, the
1st amphidicosm (Fig. 6.2(d)), actually needs to be placed *four* times to reorient
the system boundary to match the torus configuration of the modified fundamental
polygon, a property which will have significant band-structure implications. Visual
representations of this comparison of the twisted manifolds with the initial torus
can be found in Appendix 6.8.1.

### 6.3.2 Minimal Insulating Filling by Kramers’ Theorem

In Ref. 216, the authors combined an understanding of the platycosms with Kramers’
theorem to make a strong statement about space-group-symmetry-enforced obstruc-
tions to insulators occurring at specific fillings. In the following text, we reproduce
their arguments and then apply them to the restricted set of layer group systems.

For any real system with spinful electrons, there exists a time-reversal operator $T$
which squares to $-1$ and mandates, according to Kramers’ theorem, that each state
is two-fold-degenerate. Under this restriction, a periodic crystal with an odd number
of electrons $N_e$ must, independent of how its boundary conditions are applied, have
a partially filled state and therefore be a metal or a semimetal [216]. That number
of electrons can be expressed as $N_e = N_{cell}\nu$, where $N_{cell}$ is the number of unit cells
and $\nu$ is the filling per unit cell. Therefore, Kramers’ theorem can be restated as a
Figure 6.3: The Su-Schrieffer-Heeger (SSH) Model, tuned to its quantum critical point, on a periodic system. In this limit, the two sublattices are energetically identical, and are therefore related by the nonsymmorphic operation of a mirror of the $y$-direction followed by a half-lattice translation in the $x$-direction. All of the information about this system can be encoded by mandating that both sublattices live at the same potential and by replacing each site with a vector object pointing in the $\pm \hat{y}$ direction (a). When the system has an even number of sites and the boundary condition is not twisted, it lives on a cylinder (b). However, one can produce an electronically equivalent system, if the number of unit cells is large, by removing one site and twisting the axis boundary condition on the $y$ direction, which places the lattice instead on a Möbius strip. The requirement that $\nu \in 2\mathbb{Z}$ to avoid a metallic state.

Now, when the unit cell is constructed of energetically identical sites related by some spatial operation, one can consider the operation which takes you between sites as a nonsymmmorphic symmetry: a combination of a fractional lattice translation and a spatial operation. The quintessential example of a system with such a symmetry is the undimerized Su-Schrieffer-Heeger (SSH) model, which is a one-dimensional bipartite chain where the sites can be equivalently represented by a local up or down vector object (Fig. 6.3(a)). While the gapped phases of this model already have a symmmorphic mirror symmetry in the $x$ direction, its quantum critical point, reached by enforcing the same chemical potential on each sublattice, possess a
second, *nonsymmorphic* symmetry, one which relates the two sublattices by a mirror of the \( y \) direction and a half-lattice translation in the \( x \) direction.

In this limit of the SSH model, one could consider taking the final unit cell before the boundary and eliminating one of the sites. This new system with a decimated unit cell, if sufficiently large, will still be electronically equivalent to the original system as long as the boundary condition reproduces the nonsymmorphic symmetry (Fig. 6.3(b)) [216]. However, the resultant crystal now has a fractional \( N_{\text{cell}} \) (here a half integer), and therefore in this crystal, assembled with this boundary condition, Kramers’ theorem actually requires that \( \nu \in 4\mathbb{Z} \) to avoid a metallic state. Stated differently, *four-band models of this SSH model tuned to have a nonsymmorphic symmetry are obstructed from being bulk insulators at half filling*. One can consider the SSH quantum critical point as a manifestation of that obstruction.

In systems with more than one periodic direction, there can be multiple nonsymmorphic symmetries to consider. The process of decimating the final unit cell and twisting the axis boundary condition to reproduce the nonsymmorphic symmetries is in fact just a reproduction of the modding process used to generate the manifolds in Section 6.3.1. In 1D (with two-dimensional sites) with this SSH model, the decimation process reduces the underlying manifold from a cylinder to a Möbius strip \(^1\). In two and layered three dimensions, this decimation process exactly corresponds to placing the lattice onto one of the manifolds in Figures 6.1 and 6.2 respectively.

\(^1\)This SSH model uses 2D sites with one periodic dimension, making it a member of the *Frieze Groups* [87]. Like with the layer groups, Frieze group systems are allowed embedding onto manifolds with the dimensionality of their sites. If the sites were one-dimensional, everything would be trivially embedded on a circle (\( S^1 \))
With multiple nonsymmorphic symmetries, the condition for flatness is a simple check in these systems whether the product of the two symmetry operations modded out, as defined from a common origin, is itself also an inherently nonsymmorphic operation. The prefactor on the integer filling to avoid a metallic state exactly corresponds to the degree of decimation of the final unit cell, expressed as the large bold numbers in Figures 6.1 and 6.2. For reference, visual representations of this decimation process for two-dimensional lattices can be found in Appendix 6.8.1.

In the limit that interactions are weak and bands are well defined, this minimum filling corresponds to the minimum number of bands which must be tangled together, independent of any band-tuning conditions. These essential tangles of bands are bounded by two- and four-fold degeneracies that can only be moved, but not gapped, by tuning space-group-allowed hopping terms. Any band crossings on lines between these degeneracies are therefore also stuck in existence, and are also only capable of movement but not gapping. Throughout this chapter, we will relate these groupings of bands to the particular WPVZ bounds for minimal insulating filling established by combining the platycosm modding procedure with Kramers’ theorem.

Finally, WPVZ noted that in three dimensions, there are a handful of exceptions to the platycosm formulation of minimal insulating filling established by these arguments, with breakdowns occurring in some cases of multiple nonsymmorphic symmetries or because of unusual, highly degenerate points [27, 224]. However, none of these exceptions occur in the 80 layer groups, and therefore the platycosm formulation...
lation of the WPVZ bound in these systems exactly captures the filling restrictions imposed by nonsymmorphic symmetries.

In Appendix 6.8.3, we list all of the layer groups as well as their corresponding space groups, allowed manifold placements, and insulating filling restrictions.

### 6.4 Band Multiplicity and Eigenvalue Structure in the Layer Groups

In the band theory limit, the arguments made by WPVZ must still be consistent with any symmetry- or topology-related mechanism for the protection of nodal features. In three-dimensional systems with strong spin-orbit coupling, nodes such as Weyl points can be locally protected by a topological invariant [209]. However, in two dimensions with strong spin-orbit interaction, or in three-dimensional systems with a higher symmetry, the protection of nodal features is determined instead by the local symmetry eigenvalue structure of the bands. In particular, to protect a node in strong spin-orbit systems in two dimensions, the bands which cross must not share the same symmetry eigenvalues of all simultaneously compatible (i.e. commuting) symmetry operations, or in general they will anticross and form a gap.

The set of protected degeneracies in the layer groups with strong spin-orbit interaction, including both essential- and band-inversion-type nodes, is therefore entirely
determined by the kinds of allowed band multiplicities and eigenvalue structures. In this section, we review basics regarding the treatment of symmetry operators in \( k \)-space, working up to how two-fold symmetries can provide more exotic degeneracies and eigenvalue pairings.

In \( k \)-space, we can consider an operation for symmetry evaluation if the rotations, inversions, and time-reverses in it return \( k \) to itself modulo \( 2\pi \). At a generic, low-symmetry value of \( k \), only the combination of \( I \) and \( T \) can be a symmetry. If \( T^2 = -1 \), then \( \tilde{T}^2 = (I \times T)^2 = -1 \) enforces Kramers’ theorem for each value of \( k \) such that bands everywhere are two-fold-degenerate.

Other symmetries are valid along points, lines, and planes and can also lead to two- or even four-fold band multiplets. In this section, we examine the examples of band multiplicity and symmetry eigenvalue character which can locally protect a band crossing in layer group systems. We start at the time-reversal-invariant momenta and reduce symmetry from there to lines and planes. We close with a discussion of symmetry eigenvalues, working up from singly-degenerate bands to eigenvalue structures in band multiplets.

### 6.4.1 Time-Reversal-Invariant Momenta

At a Time-Reversal-Invariant crystal Momentum (TRIM), the layer groups will host symmetry-required degeneracies of 2 or 4 bands for systems with time-reversal-
symmetry $\mathcal{T}$. Kramers’ theorem requires that under $\mathcal{T}^2 = -1$, states at the TRIMs are two-fold-degenerate. Additionally, should $\mathcal{T}|u\rangle \neq \Pi|u\rangle \neq |u\rangle$, where $\Pi$ is an arbitrary symmetry operation valid at that particular TRIM, the Hamiltonian must have a degeneracy of at least 4. A common example of this relationship between $\mathcal{T}$ and $\Pi$ occurs with two-fold symmetries, for which if two spatial operations have representations which commute with time-reversal and anticommute with each other, and at least one of them squares to $+1$, then states at that TRIM will be 4-fold-degenerate. Four-fold degeneracies can also occur at points owing to the relationship between a spatial symmetry and a rotation of order $n > 2$ [24, 135], but in the layer groups, these systems are unable to host many of the essential nonsymmorphic nodal features on which this chapter focuses, and therefore we will restrict our discussion to systems with two-fold rotations.

6.4.2 Crystalline Symmetries

Away from the TRIMs, bands along lines and planes can be eigenstates of rotation, mirror, glide mirror, and screw rotation. The eigenvalues of these operations are independent of their position-space origins, though their relative commutation relations, as we will see, are not. Spatial inversion $\mathcal{I}$ ($\vec{k} \rightarrow -\vec{k}$), valid only at the TRIMs, does not involve the spin degree of freedom, and thus independent of the square of time-reversal always has eigenvalues $\pm 1$. For the remaining operations, we will restrict ourselves to the case where $\mathcal{T}^2 = -1$. Rotations about an axis ($C_{n\vec{v}}$
where the rotation is through an angle $2\pi/n$ about $\vec{v}$ have eigenvalues $(-1)^{1/n}$ and are valid along high-symmetry lines in 2D and 3D. Mirror, or an improper rotation, can be considered the product of $I$ and $C_{2v}$ and therefore has eigenvalues $\pm i$. Mirrors are valid along planes in 3D and lines in the layer groups, except for $M_\vec{z}$ which is valid for the whole 2D BZ.

A nonsymmorphic operation, a glide or a screw, can be considered as a mirror or a rotation $g$ about some point in space, followed by a fractional lattice translation $\vec{t}$ in a direction such that $g\vec{t} = \vec{t}$. They are valid along the same BZ lines and planes as are their symmorphic counterparts. For a half translation, these operations (rotation or mirror) take on the same eigenvalues as their symmorphic counterparts, $\pm i$, multiplied by $e^{i\vec{k} \cdot \vec{t}}$:

$$\lambda_{2-\text{fold } NS}^\pm = \pm ie^{i\vec{k} \cdot \vec{t}}, \quad \vec{G} \cdot \vec{t} = \pi$$ (6.4.1)

where $\vec{G}$ is a reciprocal lattice vector such that $\vec{t}$ is a half-lattice translation. In the layer groups, the consideration of nonsymmorphic symmetries is greatly simplified as there are only two-fold screws and glide mirrors; higher-fold screws or quarter-translation “d” glides require some amount of translation or rotation into the stacking or $z$ direction. At the representation level, nonsymmorphic symmetries always have the same square at $\Gamma$ as their symmorphic counterparts, a value which winds by $-1$ as one moves along the half-translation direction in the BZ.
As highlighted in Ref. 245, the fractional translation of a nonsymmetric symmetry gives the nonsymmetric eigenvalues a $k$ periodicity greater than the $2\pi$ of the Brillouin zone. For a half translation, the eigenvalues wind with a $4\pi$ periodicity, which dictates that the $+$ and $-$ eigenstates of a glide or a two-fold screw have to connect somewhere along the translation direction and resolve this discrepancy. In fact, this implies that the choice of designating a band as a $+$ or $-$ eigenstate away from $\Gamma$ is a gauge choice, as the eigenvalues cannot be defined continuously and with period $2\pi$.

This inability to define a $2\pi$-periodic gauge for nonsymmetric symmetries, and the resolution that bands are required to cross, is in fact the band-theory limit of the WPVZ bound on the minimal insulating filling. For all two-fold nonsymmetric systems, bands can be found in groupings of no fewer than 4, and so at fillings other than $4\mathbb{Z}$, these systems are unavoidably metallic. Furthermore, even when nodal features at fillings $\nu \neq 4\mathbb{Z}$ have well-defined topological indexes, such as Chern numbers for Weyl points in three dimensions, this requirement that 4 or more bands must be tangled together in two-fold nonsymmetric systems obstructs two nodes from combining and gapping out. As we will see in the examples throughout this chapter, even if two Weyl points have opposite Chern numbers, they may not be pairwise eliminated if they are part of a nonsymmetric-symmetry-enforced tangle of bands.
Figure 6.4: Possible locations of a glide line $G_y$ relative to an inversion center $I$ (⊗) in a 2D rectangular system with TRIMs $\Gamma XMY$. In both cases, for $\mathcal{T}^2 = −1$ all states are two-fold-degenerate because there is a local time-reversal operator $(\mathcal{IT})^2 = −1$. If the inversion center is coincident with the glide line (a), there will be four-fold representations at $X$ and $M$, but all eigenstates of $G_y$ will have eigenvalue pairings $\{+,−\}$ and can never cross. If the inversion center differs from the glide line by a quarter-lattice spacing $a_y/4$ (b), then the operator for $G_y$ will contain an extra $t_y/2$ when defined from the common origin of the inversion center, leading to four-fold points instead at $X$ and $Y$. In this case, then while the bands along $\Gamma X$ are still paired with $G_y$ eigenvalues $\{+,−\}$, bands along $YM$, if two-fold-degenerate, will be characterized by $G_y$ eigenvalue pairings $\{+,+\}$ or $\{-,−\}$ and can cross and create four-fold Dirac points with local protection [56].
6.4.3 Two- and Four-Fold-Degenerate Band Multiplets

If bands are singly degenerate, then the determination of their symmetry eigenvalues for all simultaneously compatible symmetry operations is sufficient for 2D systems with strong spin-orbit interaction in determining if bands can cross and form locally-protected nodal features. However, when bands are two- or four-fold-degenerate, then one additionally has to determine the symmetry eigenvalues of all bands in the multiplet. Absent the consideration of rotations of order \( n > 2 \), a two-fold-degenerate state can occur at a point if either the representations of two spatial operations valid at that point anticommute, or if the combination of a spatial operation \( \Pi \) and \( \mathcal{T} \) return \( \mathbf{k} \) to itself at that point and \( (\Pi \times \mathcal{T})^2 = -1 \), locally enforcing Kramers' theorem. In the layer groups, two kinds of spatial operations \( \Pi \) support these conditions: spatial inversion \( \mathcal{I} \) and two-fold nonsymmorphic symmetries.

When the center of inversion \( \mathcal{I} \) lies on all mirror and rotation lines, this picture is greatly simplified. Taking \( G_y = t_{x/2} M_y \) on a 2D rectangular lattice as an example, we can first consider the case where the inversion center is coincident with the glide line (Fig. 6.4(a)). Because both \( \mathcal{I} \) and \( \mathcal{T} \) flip \( \mathbf{k} \) and \( \mathcal{I}^2 = +1 \), all bands will be two-fold-degenerate for strong spin-orbit systems where \( \mathcal{T}^2 = -1 \). However, to evaluate the potential semimetallic properties of this geometry, it is necessary to determine the \( G_y \) eigenvalue structure of the bands along \( \Gamma X \) and \( Y M \), as well as the locations of any required four-fold-degenerate points. We can examine the relationship between \( \mathcal{I} \), \( \mathcal{T} \), and \( G_y \) as representations on a four-site \( \mathcal{H}(\mathbf{k}) \) and use the
additional factors of $e^{i \vec{k} \cdot \vec{r}}$ from the full lattice translations $\vec{r}$ to establish commutation relations. Calling the representation of the operator for this case of inversion center location $G_y^a$, at a TRIM:

$$G_y^a \mathcal{I} = t_{x/2} M_y \mathcal{I}$$

$$= \mathcal{I} t_{-x/2} M_y$$

$$= t_x t_{x/2} M_y$$

$$G_y^a \mathcal{I} = e^{-i k_x} \mathcal{I} G_y^a$$

(6.4.2)

where in the final line we have acted $t_{-x}$ on an eigenstate of $G_y$. For mathematical consistency, it was crucial that we have chosen all operations to have the same position-space origin (here the inversion center). Though this nuance can be overlooked when all mirror planes and lines are coincident with the inversion center, as they are in Ref. 245, it becomes a central detail when evaluating the eigenvalue character of systems for which one is unable to define a common origin for two spatial symmetries, as we will see throughout this chapter. Equation 6.4.2 implies that $\{G_y^a, \mathcal{I}\} = 0$ at $X$ and $M$. As $\mathcal{I}^2 = +1$ at those points, the emphasized statement in 6.4.1 implies that representations at those TRIMs must be $4 \times 4$, and thus that all states at $X$ and $M$ are four-fold-degenerate (Fig. 6.4(a)).

Away from the TRIMs, we must additionally determine the $G_y$ eigenvalues of
bands along glide lines. Considering \( |+\rangle \) to be the positive eigenstate of \( G_y \) such that:

\[
G_y^a|+\rangle = ie^{ik_x/2}|+\rangle \tag{6.4.3}
\]

whose eigenvalue we compare to the local Kramers partner \( \mathcal{IT}|+\rangle \):

\[
G_y^a(\mathcal{IT}|+\rangle) = t_x/2 M_y \mathcal{IT}|+\rangle \\
= \mathcal{IT} t_{-x/2} M_y |+\rangle \\
= t_x \mathcal{IT} G_y^a |+\rangle \\
G_y^a(\mathcal{IT}|+\rangle) = -ie^{ik_y/2} (\mathcal{IT}|+\rangle) \tag{6.4.4}
\]

revealing that along both \( \Gamma X \) and \( Y M \) all two-fold-degenerate bands have \( G_y \) eigenvalues \{+,−\} and thus can only anticross (Fig. 6.4(a)).

However, as emphasized in Ref. 56, this picture changes significantly when the inversion center does not lie along a particular glide line or screw axis. Consider a 2D rectangular system with a glide line \( G_y = t_x/2 M_y \) that lies \( a_y/4 \) above the inversion center (Fig. 6.4(b)). In order to consistently keep the commutation relations of the representations \( [\mathcal{I}, M_i] = 0 \) and \( \{C_{2i}, C_{2j}\} = -2\delta_{ij} \) (true for spinful systems where
\[(C_{2i})^2 = -1\), we have to define at the operator level:

\[G_y^b = t_y/2 t_x/2 M \hat{y}\]  

(6.4.5)

where \(G_y^b\) will here indicate a glide that lies a quarter-lattice \(y\)-direction displacement from the inversion center. Reevaluating the commutation relations at the TRIMs:

\[G_y^b I = t_y/2 t_x/2 M \hat{y} I = I t_x/2 t_y/2 M \hat{y} = t_x t_y I t_x/2 t_y/2 M \hat{y} = e^{-ik_x} e^{ik_y} \mathcal{I} C_y^b\]  

(6.4.6)

where the final line is evaluated by acting the translations on an eigenstate of \(G_y\). In this case, \(\{G_y^b, \mathcal{I}\} = 0\) now at \(X\) and \(Y\), which by the arguments in 6.4.1 requires that all states be four-fold-degenerate at those TRIMs (Fig. 6.4(b)).

Moving off of the TRIMs, we can examine how this inversion-center offset affects the eigenvalue character of the local Kramers partners:
This implies that along $\Gamma X$, two-fold-degenerate bands still have $G_y$ eigenvalue pairings $\{+,-\}$ and still always anticross. But along $Y M$, if states are two-fold-degenerate, they will have $G_y$ eigenvalues $\{+,+\}$ or $\{-,-\}$, and along that glide line a four-fold crossing can therefore be locally protected (Fig. 6.4) [56]. However, 

we have not specified whether such a crossing must occur, as is required for example in SrIrO$_3$ in space group 62 [34]. Such a distinction requires additional information about the nonsymmorphic symmetries present globally across the BZ. In subsequent sections, we will provide both examples of layer group systems where four-fold crossings protected by an inversion-center offset are required in essential semimetals and optional in band-inversion semimetals.

Two-fold-degenerate lines and planes can also occur in systems with two-fold nonsymmorphic symmetries [54, 224]. For example, in a rectangular two-dimensional system, the product of $\Pi = t_x/2 M_y$ and $\mathcal{T}$ returns $\vec{k}$ to itself along $\Gamma Y$ and $X M$. Independent of $\mathcal{T}^2$, $(\Pi \mathcal{T})^2 = t_x e^{ikx}$ when acted on a state, guaranteeing states
are at least two-fold-degenerate along $\overline{X\overline{M}}$ where $(\Pi T)^2 = -1$. In these systems, bands along this line can be two-fold-degenerate and, as was the case with inversion symmetry, can be paired with either the same or the opposite eigenvalues of another symmetry operation valid along that line, depending on the relative origins of the crystalline symmetries. This can, in at least the case of breaking a double Dirac point in space group 135, lead to an unusual Dirac semimetal without inversion symmetry [224]. In the 2D cases of the layer groups, there may not be enough degrees of freedom to create a system without inversion where such four-fold-degenerate crossings are the only features at the Fermi energy.

Four-fold-degenerate lines are also occasionally possible in the layer groups. For example, consider a system where along a line two crystalline symmetries $\Pi_1$ and $\Pi_2$ are valid and bands are already required to be two-fold-degenerate either by inversion and $T^2 = -1$ or by a two-fold nonsymmorphic symmetry. If $|+\rangle_1$ has the same $\Pi_1$ eigenvalue as its local Kramers partner and if $\{\Pi_1, \Pi_2\} = 0$ along this line, then that guarantees that $\Pi_1|+\rangle_1 \neq \Pi_1\Pi_2|+\rangle_1$. Therefore bands along the line are four-fold-degenerate with $\Pi_1$ eigenvalues $\{+, +, -, -\}$.

However, as exhaustively detailed in Ref. 26, a system can only host one four-fold irreducible representation along a line in three dimensions, and therefore also in layer group systems. Two four-fold-degenerate lines can thus never cross to form a locally-protected eight-fold-degenerate point along a line in three or fewer dimensions.
6.5 Semimetals in the Layer Groups

Seeking to examine nodal phenomena from both WPVZ bound and crystalline symmetry perspectives in strong spin-orbit systems in the layer groups, we present a simple model that typifies the layer group systems which contain essential or notable band-inversion nodal features. In this section, we show how a four-site rectangular lattice can capture a large variety of both essential and band-inversion semimetallic features in two dimensions when its sites are dressed with three-dimensional vector objects, which one can think of as local displacements or dipole moments. After presenting this construction, we present models for 7 specific layer groups, which represent all possible essential semimetallic features in the layer groups, as well as relevant related examples of band-inversion nodal features. We sort our models by their WPVZ bounds in the platycosm formulation, and show using local eigenvalue character how nodal features are protected. Finally, we show how some of these quasi-two-dimensional systems relate to existing three-dimensional semimetals.

As seen in Figure 6.5, our model system consists of four sublattices arranged on a rectangular lattice. Describing our sublattice space with Pauli matrices, $\tau^x$ describes s-orbital-like hopping between the A and B sites and $\mu^x$ describes s-orbital-like hopping between the A and C sites, such that second-neighbor s-like hopping is given by $\tau^x \mu^x$. Each site also has a spin degree of freedom $\sigma$ which is flipped under time-reversal $T = i\sigma_y K \otimes (\vec{k} \rightarrow -\vec{k})$ for a general $\mathcal{H}(\vec{k})$. This four-site unit cell, like that of any crystal system with multiple sites per unit cell, can be viewed as
originating from a parent high-symmetry Bravais lattice, here a rectangular lattice with spherical sites. Applying a time-reversal-symmetric tensor field (like an electric field) lowers the periodicity of the system and breaks some subset of point group symmetries at each site \(^2\). Our model can be realized by choosing just a dipole vector field, such that each site is dressed with a three-dimensional vector object that encodes the underlying crystal symmetries. Physically, this vector can be considered as a local displacement of a single atom or a dipole moment between two atoms.

As one can observe by perusing the table in Appendix 6.8.3, layer groups with \(C_{3\hat{z}}\) or \(C_{6\hat{z}}\) symmetries can only achieve WPVZ bounds of 2, owing to their inability to

\(^2\)Choosing a time-reversal-breaking field, such as a pseudovector magnetic field, is also allowed. Instead of generating the 230 space groups, this leads rather to the 1651 magnetic space groups [128].
host nonsymmorphic symmetries. While these systems can host rotation-protected band-inversion type semimetals, they will not be the focus of this chapter. One could consider a system with \( C_{4z} \) symmetry as a limiting case of the lattice in Figure 6.5, in which case our model would collapse onto a version of the model in and recapture the physics of Ref. 245.

Setting first all of the site vectors to \( \vec{0} \), we can write down a very high-symmetry Hamiltonian consisting of all possible s-orbital-like hoppings between first- and second nearest neighbors:

\[
\mathcal{H}_0 = t_x \cos \left( \frac{k_x}{2} \right) \tau^x + t_y \cos \left( \frac{k_y}{2} \right) \mu^x \\
+ t_2 \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) \tau^x \mu^x \tag{6.5.1}
\]

where we have set the lattice constants \( a_x = a_y = 1 \) and enforce the inequivalence between \( x \) and \( y \) by keeping \( t_x \neq t_y \). As the on-site vectors are turned on, new hopping terms are allowed, and the symmetry is reduced into a particular layer group. For a given layer group \( LG \), the full second-neighbor Hamiltonian \( H_{LG} = H_0 + V_{LG} \), where \( V_{LG} \) contains all of the layer-group-specific hopping terms beyond Eq. 6.5.1. The details of deriving \( V_{LG} \) for each of our examples, as well as layer-group-specific expressions for it, are noted in detail in Appendix 6.8.2.
As detailed earlier in 6.3.1, by allowing placement onto at least one of the four platycosms in Figure 6.2, layer group systems can achieve WPVZ bounds of 2, 4, or 8, and will therefore host corresponding numbers of inseparably tangled bands. Within the systems with WPVZ bounds of 2 and 4, band-inversion metallic and nodal features are also possible for this eight-band model. In the following sections, we present typifying examples for layer group semimetals within each possible WPVZ bound, showing for each example how the WPVZ bound relates to the more familiar crystalline symmetry analysis.

### 6.5.1 WPVZ Bound of 2

Without the presence of a nonsymmorphic symmetry, only time-reversal symmetry can force bands to group together [216, 244, 245]. Layer groups with only symmorphic symmetries have band structures with two-fold degeneracies at the time-reversal-invariant momenta when $\mathcal{T}^2 = -1$. Therefore, at even fillings, any such system with more than two bands can either be an insulator or a band-inversion semimetal. In the layer groups, there are myriad ways for a band-inversion crossing to be locally protected by mirror or rotation eigenvalues, so we will only explore one such example in a system with singly-degenerate bands.

To start, consider a simple system for which the $xy$-plane itself is a mirror, such that all bands have good $M_\hat{z}$ quantum numbers. For real materials this corresponds to a system which is not buckled or has no additional stacking or external field
Layer Group 37 (Space Group 47)

(a) \[ \vec{v}_A = \{M_\hat{x}|\frac{1}{2} 0\}, \{M_\hat{y}|0 \frac{1}{2}\}, \{M_\hat{z}|0 0\} \]

(b) \[
\begin{array}{cc}
\text{C} & \text{D} \\
\text{A} & \text{B}
\end{array}
\]

(c) 

Figure 6.6: The generators (a), lattice (b), and a typical band structure (c) for \textit{pmmm}, layer group 37, (space group 47). All elements of the layer group are symmorphic, with mirror lines separating the A and B sublattices and the A and C sublattices. As the \textit{xy}-plane itself is a mirror, this system is flat and has inversion symmetry, with the inversion center lying at the center of the four sites and at the intersection of all 3 mirror lines and planes. Therefore, by the arguments in 6.4.3, bands are two-fold-degenerate with \( M_\hat{z} \) eigenvalues \{+,-\}. Consequently, the bands can only anticross, and at even fillings this system is always an insulator (c).

structure which distinguishes \( \pm \hat{z} \), such as graphene without a substrate.

Restricting ourselves to one of these flat layer groups, layer group 37 \textit{pmmm} (which when stacked, is equivalent to space group 47), we first choose an example with only symmorphic symmetries, and therefore a WPVZ bound of 2. The presence of inversion symmetry \( \text{I} \), combined with time-reversal makes all bands two-fold-degenerate (Fig. 6.6). The inversion center lies at the intersection of all three mirror lines and planes (Fig. 6.6(b)), and therefore all states and their local Kramers partners have opposite \( M_\hat{z} \) eigenvalues, as detailed in 6.4.3 and Ref. 56. Therefore, regardless of band-tuning conditions, this system will generically be an insulator, because nearby bands can only anticross (Fig. 6.6(c)).
Figure 6.7: The generators (a), lattice (b), and a typical band structure (c) for \textit{pmm2}, layer group 23, (space group 25). All elements of the layer group are symmorphic, with mirror lines separating the A and B sublattices and A and C sublattices. The vectors have been bent up into the $+\hat{z}$ direction, breaking $M_\hat{z}$ as one would see if there were a substrate or a perpendicular electric field added to a system in layer group 37 (Fig. 6.6). Consequently, this system is also a \textit{wallpaper group}, and could describe the surface of a three-dimensional object. Without inversion, nonsymmorphic symmetries, or $n > 2$ $C_n\hat{z}$ rotation points, bands are singly degenerate and can only cross with local protection by mirror eigenvalues on the mirror lines. Typical values of the tight-binding parameters give metallic states at half-filling (c), but values can also be chosen to separate the bands into groups of two and open up consistent gaps at all even fillings (d).
Conversely, one could imagine putting on an electric field, like that of a substrate, which bends the on-site vectors out of the plane in the $+\hat{z}$ direction. As shown in Figure 6.7, this reduces the layer group to 23 $pmm2$ (space group 25) and breaks $M_\hat{z}$ and $I$, allowing for new first- and second-nearest-neighbor hopping terms. As this layer group only consists of in-plane mirrors and rotations about the $z$ axis, it is also one of the wallpaper groups described in 6.3.1 and could be constructed in purely two dimensions, for instance as the surface of a three-dimensional object. Bands in this layer group are now singly degenerate, and therefore have the ability to cross with local protection. Consider tuning the tight binding parameters for this layer group to roughly physical values, such that first-neighbor hopping terms are larger than second-neighbor ones and s-orbital-like hopping terms are larger than the terms for spin-orbit interaction. For these typical values of the tight-binding parameters, this system is a band-inversion semimetal (Fig. 6.7(c)). However, values could also be chosen to open up gaps at all even fillings (Fig. 6.7(d)), because in this layer group, the WPVZ bound only requires that bands tangle together in groups of 2.

### 6.5.2 WPVZ Bound of 4

A layer group system with one or more two-fold nonsymmmorphic symmetries is allowed placement onto a platycosm other than the 3-torus, and it will therefore host essential groupings of four or eight bands [216]. Within systems with a WPVZ
Layer Group 44 (Space Group 55)

(a) \[ \vec{\nu}_A = \{C_{2x} | \frac{1}{2} 0\}, \{C_{2y} | 0 \frac{1}{2}\}, \{M \hat{z} | 0 0\} \]

(b) \[ A \quad C \quad \begin{array}{c} \downarrow \end{array} \quad \begin{array}{c} \uparrow \end{array} \quad D \]

\[ \begin{array}{c} \uparrow \end{array} \quad \begin{array}{c} \downarrow \end{array} \quad A \quad \begin{array}{c} \uparrow \end{array} \quad \begin{array}{c} \downarrow \end{array} \quad B \]

Figure 6.8: The generators (a), lattice (b), and a typical band structure (c) for \textit{pbam}, layer group 44, (space group 55). This group is a flat layer group generated by constraining into the \textit{xy}-plane a system generated by two perpendicular screws. Consequently, it has inversion symmetry, with the inversion center located in the center of the unit cell, off of the glide lines resulting from the product of \( \mathcal{I} \) and \( S_{2x/y} = t_{x/y/2}C_{2x/y} \). All bands are at least two-fold-degenerate by \( (\mathcal{I}\mathcal{I})^2 = -1 \) and bands along XKM and YKM are four-fold-degenerate by the combination of glide mirror and \( M \hat{z} \), as detailed in 6.4.3. Bands at X, Y, and M are four-fold-degenerate due to the relationship between \( \mathcal{I} \) and \( S_{2x/y} \), as detailed in 6.4.1 and Ref. 245, and disperse linearly. Therefore, at fillings of \( \nu = 2, 6 \), this system is an essential Dirac line node semimetal. Two-fold-degenerate bands are all paired with \( M \hat{z} \) eigenvalues \{+, -\} or in four-fold multiplets with \( M \hat{z} \) eigenvalues \{+, +, -, -\}, and therefore cannot be tuned to cross by band inversion. Consequently, at half filling (\( \nu = 4 \)), this system is necessarily an insulator.
bound of 4, band-inversion semimetals are still possible between groupings of 4 bands, though if bands are two-fold-degenerate, additional conditions are required for determining if band inversions can be locally protected by eigenvalue character. In this section, we first examine two layer groups with WPVZ bounds of 4, which at fillings of $\nu = 2, 6$ are essential semimetals with Weyl or Dirac features, as explored in Ref. 245. After, we present an example of a band-inversion Dirac semimetal at half filling, protected locally by the inversion-center-offset arguments in 6.4.3 and Ref. 56.

We start with a high-symmetry flat system in layer group 44 \textit{pbam} (space group 55) (Fig. 6.8). This group is generated by two perpendicular screws protruding from the sites enforced in combination with $M\hat{z}$, such that the site vectors are confined in the $xy$ plane (Fig. 6.8(a)). For determining the WPVZ bound, one could either choose a screw and mod out onto the dicosm, or combine a screw with $M\hat{z}$ to create a glide line and mod out onto the 1st amphicosm:

$$t_{x/2}C_{2x}M\hat{z} = t_{x/2}C_{2x}IC_{2z} = -it_{x/2}IC_{2y} = -i(t_{x/2}M\hat{y}) \quad (6.5.2)$$

where we have used the fact that in spinful systems the representations of two-fold rotations obey the same algebra as the Pauli matrices. Either choice of manifold results in a WPVZ bound of 4, a property clearly visible by noting the gap at $\nu = 4$ in the band structure (Fig. 6.8(c)).
Due to the relationship between two-fold nonsymmorphic symmetries and inversion, highlighted in 6.4.1 and Ref. 245, the TRIMs at the end of the translation directions (X, Y, and M) all host four-fold degeneracies. All bands are at least two-fold-degenerate with pairs of opposite $M_\hat{z}$ eigenvalues. Bands along $XM$ and $YM$ have the requisite offset from the inversion center to have screw eigenvalues $\{+, +\}$, but due to the additionally valid $M_\hat{z}$ are four-fold-degenerate with mirror eigenvalues $\{+, +, -, -\}$, as detailed in 6.4.3, and are thus unable to cross. Therefore, at half filling ($\nu = 4$), this system is always an insulator. Observing symmetry-allowed terms in the tight-binding model in Appendix 6.8.2, all four-fold points and lines disperse linearly, and therefore at fillings of $\nu = 2, 6$ this system is an essential Dirac line node semimetal.

We can locally break $M_\hat{z}$ on the A site and then use the same screws as generators to produce layer group 21 $p2_12_12$ (space group 18) (Figure 6.9). In this system, bands are now singly degenerate, except along $XM$ and $YM$ where they are paired by the combination of $\mathcal{T}$ and a two-fold nonsymmorphic symmetry, as detailed in 6.4.3. As verified by analysis of symmetry-allowed linear terms in the tight binding model in Appendix 6.8.2, bands along $\Gamma X$ and $\Gamma Y$ feature essential 2D Weyl points and form essential 4-band tangles which resemble hourglasses [245]. As noted in 6.4.2, these points cannot be paired at any of the TRIMs and eliminated as long as the two screws are preserved, as the combination of the nonsymmorphic symmetry and $\mathcal{T}^2 = -1$ provides a topological obstruction to doing so, even when this system is stacked into the third dimension and the Weyl points become 3D with
Layer Group 21 (Space Group 18)

(a) \( \vec{v}_A = \{C_{2x} | \frac{1}{2} 0\}, \{C_{2y} | 0 \frac{1}{2} \} \)

(b) A C B D

(c) 

Figure 6.9: The generators (a), lattice (b), and a typical band structure (c) for \( p2_1 \overline{2} \overline{1} \), layer group 21, (space group 18). This low-symmetry group is generated just by two perpendicular two-fold screws protruding from the sites. Due to having broken inversion symmetry and a combination of nonsymmetric symmetries incompatible with placement onto the 1st amphidicosm in Fig. 6.2, this system has essential 4-band tangles which resemble hourglasses, such that at fillings of \( \nu = 2, 6 \), it has 2D essential Weyl points along \( \Gamma Y \) and \( \Gamma X \) \[245\]. Bands along most lines are singly degenerate and therefore capable of crossing with symmetry protection by the same mechanism as in Fig. 6.6 (though for the choice of parameters in (c) the system is an insulator at half filling; \( \Gamma Y \) is narrowly gapped). Bands along \( XM \) and \( YM \) are two-fold-degenerate by the combination of a two-fold nonsymorphic symmetry and \( T \), as detailed in 6.4.3. M hosts four-fold points despite the absence of inversion, owing to \( \{S_{2x}, S_{2y}\} = 0 \) and \( (S_{2x})^2 = (S_{2y})^2 = +1 \) at this point, as detailed in 6.4.1. At fillings of \( \nu = 2, 6 \), this system is therefore an essential semimetal, and can be tuned to have a minimal Fermi surface of four Weyl points and a Dirac point.
well-defined Chern numbers. At M, the two screws anticommute and square to +1, and therefore despite the absence of inversion symmetry, bands at M are four-fold-degenerate, and in fact are linearly dispersing. Therefore, at fillings $\nu = 2, 6$, this system is an essential point node semimetal, and can be tuned to have a minimal Fermi surface of four Weyl points and a Dirac point. Though we have chosen parameters which gap this system at half filling (Fig. 6.9(c)), the singly-degenerate bands across many of the high-symmetry lines are capable of inverting with local protection by the same mechanism as a previous system with a WPVZ bound of 2, layer group 23 (Fig. 6.7).

It is worth noting that despite having two perpendicular nonsymmorphic symmetries, layer groups 44 and 21 do not achieve WPVZ bounds of 8. One can understand this bound limitation by recalling that a key requirement of the modding procedure in 6.3.1 was the selection of manifolds without fixed points. In terms of symmetry operations, this requirement can be restated, as noted by Bieberbach, that the product of the nonsymmorphic symmetries selected for modding, as defined from a common origin, must itself also be a nonsymmorphic operation [89]. Examining the two screw generators:

$$t_x/2C_2xt_y/2C_2y = i t_x/2t_{-y/2}(C_{2z})$$

(6.5.3)

which is itself just a $C_{2z}$ symmorphic rotation about the center of the unit cell.

228
As we will see in the subsequent section, the only combination of operations which can achieve a WPVZ bound of 8 in layer group systems is \( t_{x/2} M_z \) and \( t_{y/2} C_{2y} \).

Within the layer groups with WPVZ bounds of 4, one can also achieve a Dirac semimetal at fillings \( \nu \in 4\mathbb{Z} \) through a band inversion transition. In \( p2_1/b11 \), layer group 17, (space group 14) (Fig. 6.10), there exists an offset between horizontal glide lines, which connect adjacent sites A and B, and inversion centers, which lie between sites A and C (Fig. 6.10(b)). As explained in Ref. 56 and in 6.4.3, this offset allows bands along \( YM \) to be two-fold-degenerate with pairs of the same glide mirror eigenvalue. At fillings \( \nu = 2, 6 \), the tight-binding models in Appendix 6.8.2 show that this system is an essential Dirac semimetal with Dirac points at \( X \) and \( Y \), but also show that other nodal features are possible at \( \nu = 4 \). A band inversion about a TRIM, here \( M \), leads to the creation of a Dirac point along \( YM \) and its time-reverse (Fig. 6.10(d)).

In a three-dimensional stack of this system, this feature would instead emerge as a Dirac line node. However, unlike the Dirac line node in SrIrO\(_3\) in Ref. 34, which is also locally protected by an inversion-center offset and a glide mirror, this line node in space group 14 could be removed by a band-inversion transition. As we will examine in the next section, SrIrO\(_3\) in space group 62 has a WPVZ bound of 8 and is in fact more closely related to a different layer group. Therefore, we find that for the protection of essential 8-band Dirac nodal features such as the line node in SrIrO\(_3\), the statements from Ref. 56 are necessary for local protection, but insuf-
Layer Group 17 (Space Group 14)

(a) \[ \mathbf{v}_A = \{I|0 \frac{1}{2}\}, \{M_y| \frac{1}{2} 0\} \]

(b) A

C

B

D

Figure 6.10: The generators (a), lattice (b), and two possible band structures (c,d) for \textit{p}2_1/b11, layer group 17, (space group 14). The lattice has horizontal glide lines along the sites and inversion centers between the A and C sites and between the B and D sites. Due to the combination of \( I \) and \( T \), bands everywhere are two-fold-degenerate. The offset between the inversion centers and the glide lines leads to four-fold degeneracies at \( X \) and \( Y \), as noted in Fig. 6.4 and in 6.4.3. As these four-fold points are linearly dispersing, in accordance with the WPVZ bound this system is an essential Dirac semimetal at fillings of \( \nu = 2, 6 \), allowing an idealized Fermi surface consisting of two Dirac points. At half filling, however, this system is capable of being both an insulator (c) or a semimetal (d), as bands along \( Y \) are two-fold-degenerate with pairs of the same glide mirror eigenvalue. This semimetallic phase is locally protected by the statements in Ref. 56, but can be gapped out by a band-inversion transition. Therefore, for guaranteeing the existence of an essential 8-band Dirac semimetallic phase, like that in SrIrO\(_3\) in Ref. 34, we find the inversion-center offset highlighted in Ref. 56 to be a necessary, but insufficient condition, and that we must require additional constraints.
ficient for guaranteeing existence. As we will explore in the following section, an inversion-center offset from a nonsymmorphic symmetry is only one of three conditions required to form an essential Dirac line node. In fact, we will see that 8-band essential semimetallic structures can even be formed in the absence of inversion symmetry.

6.5.3 WPVZ Bound of 8

Though many layer groups exist with multiple perpendicular, two-fold nonsymmmorphic symmetries, only 3 such groups exist which satisfy the condition for modding out more than one nonsymmmorphic operation, namely that the product of the two operations, as defined from a common origin, is itself also a nonsymmmorphic operation [89]. We find that in the 80 layer groups, only groups with both \( t_{x/2}M_z \) and \( t_{y/2}C_{2y} \) (as well as any trivial, in-plane rotations of them) can achieve this condition and therefore allow placement onto the 1st amphidicosm and have WPVZ bounds of 8.

Of these three layer groups, two of them, layer groups 43 and 45, have inversion symmetry and are very similar to each other. Choosing to focus on the high-symmetry layer group 45, \( pbma \) (Fig. 6.11), we can see clearly along \( X \overline{M} \) a robust 8-band Dirac feature which matches the nodal ring in \( \text{SrIrO}_3 \) [34] (Fig. 6.11(c)). In fact, space group 57, the stacked equivalent of layer group 45, is closely related to the \( \text{SrIrO}_3 \) \( pbnm \) space group 62, with the chief difference coming from the substitution
Layer Group 45 (Space Group 57)

(a) \( \vec{v}_A = \{M_\frac{1}{2} \mid 0\}, \{C_{2y} \mid \frac{1}{2} \frac{1}{2}\}, \{I \mid \frac{1}{2} \frac{1}{2}\} \)

(b) A C B D M X

{++++} {----} {++--} {++--}

(d)

Figure 6.11: The generators (a), lattice (b), and a typical band structure (c) for \textit{pbma} layer group 45 (space group 57). This high-symmetry layer group has glide mirrors in the \( x \) and \( z \) directions and \( M_y \) about the sites, such that it has an inversion center in the center of its unit cells, off of glide line \( G_x = t_y/2 \). This offset allows for bands along \( XM \) to be two-fold-degenerate with the same \( G_x \) eigenvalues, which locally protects Dirac points along that line and its time-reverse, much like the local protection of the Dirac point in Fig. 6.10(d). However, unlike in that previous semimetal, whose nodal features were optionally created by tuning through a band-inversion transition, the Dirac points in layer group 45 are \textit{essential}, making them more like the essential Dirac line node in \textit{SrIrO}_3 in space group 62 [34]. Because four-fold points are required at \( X \) and \( M \) by the relationship between \( G_x, S_y = t_{x/2}t_{y/2}C_{2y}, \) and \( I, \) and because \( G_x \) commutes with all other independent symmetry operations of the layer group at \( M \), four-fold points at \( X \) and \( M \) have differing \( G_x \) eigenvalue pairings (d), leading to the required crossing along \( M\overline{X} \).
of a three-dimensional “n-glide” with an in-plane “b-glide”.

The relationship between layer group 45 and space group 62 can be examined both from a consideration of allowed flat manifold placements and from an evaluation of band multiplicity and symmetry eigenvalue structure. In the language of WPVZ, layer group 45 (space group 57) has a four-site unit cell with nonsymmorphic symmetries $t_{x/2}M_z$ and $t_{y/2}C_{2y}$ as defined from the common origin of the midpoint between the A and B sites, leading as explained in 6.3.1 to an allowed placement onto the 1st amphidicosm and the requirement that at least 8 bands be tangled together. Space group 62 has a four-site unit cell with its $S_y$ above the glide plane, so using the same axes one can mod out the nonsymmorphic operations $t_{x/2}M_z$ and $t_{z/2}t_{y/2}C_{2y}$, allowing placement onto the 2nd amphidicosm and requiring that at least 8 bands be tangled together (the 2nd amphidicosm is a fundamentally three-dimensional manifold and does not neatly decompose into the modified fundamental polygons from Fig. 6.2.) Finally, as neither space group 57 nor space group 62 is among the 10 known space groups for which the platycosm formulation of the WPVZ bound is insufficient, we can deduce that in these two space groups all minimally tangled bands will in fact come in groups of exactly 8 [216].

From a symmetry perspective, the story regarding this band structure is a bit more involved. We find that there are three criteria which must all be met to guarantee the existence of an essential eight-band tangle in an orthorhombic system with inversion symmetry. First, one must check whether or not any two-fold
nonsymmorphic symmetry lines or planes exist offset from an inversion center. As detailed in 6.4.3 and Ref. 56, a system which fulfills this criterion, if it has two-fold-degenerate bands along the \( k \)-space nonsymmorphic line or plane at the zone boundary, will have multiplets with the same eigenvalue of the nonsymmorphic symmetry that can cross and form Dirac points with local protection. The second criterion involves checking whether such a crossing is prohibited from being removed by a band-inversion transition. Such a process can only be prevented when bands at the TRIMs on either side of the two-fold nonsymmorphic line or plane, here at \( M \) and at \( X \), are all four-fold-degenerate. Determining this degeneracy can either be accomplished by considering at those TRIMs the algebra between all of the independent space group generators, or by consulting a crystalline symmetry textbook such as Bradley and Cracknell [26]. Finally, and most importantly, to prove that an odd number of Dirac crossings must exist along the high-symmetry line, one must additionally show that the four-fold-degenerate bands at the bounding TRIMs support a particular algebra. Specifically, at the TRIM where the nonsymmorphic operation which is offset from the inversion center squares to +1, that symmetry must commute with all other independent operations which generate the space group and are valid at that TRIM. If this final criterion is met, then the nonsymmorphic operation must have at that point, here \( M \), a \( 4 \times 4 \) representation proportional to the identity and therefore eigenvalues \{+,+,+\} or \{-,-,-,\}. As at the other bounding TRIM where the nonsymmorphic operation squares to -1, here \( X \), time-reversal requires that the imaginary nonsymmorphic eigenvalues be paired
\{+,-,+,-\}, doubly-degenerate bands must cross an odd number of times between the two bounding TRIMs and form at least one essential Dirac crossing. In three dimensions, if this occurs in a glide plane, then any path between the two TRIMs must contain a Dirac crossing and a Dirac line node forms, as is the case in SrIrO$_3$.

Elements of these criteria for this particular iridate system were recently noted in Ref. 40.

Returning to layer group 45, we can examine how evaluating these criteria works in practice. Only the product of two generators, $G_x = t_{y/2}M \hat{z}$, satisfies the inversion-center-offset criterion and is therefore suitable for consideration. Bands at $X$ must be four-fold-degenerate, as $\{G_x, I\} = 0$ here and $I^2 = +1$, as noted in 6.4.1. At $M$, another two-fold operation, such as $t_{y/2}C_{2y}$, as defined from an inversion center, can anticommute with one of the two remaining independent layer group generators and mandate that bands there also be four-fold-degenerate. Finally, we can note that as defined from a common origin along the $G_x$ lines, $[G_x, \Pi] = 0$ at $M$ for all $\Pi$, where $\Pi$ is an independent generating operation of layer group 45. Matching bands with the same $G_x$ eigenvalues $\lambda^\pm = \pm ie^{ik_y/2}$, Fig. 6.11(d) shows that these criteria necessitate the existence of a Dirac point along $XM$.

While more involved than the WPVZ bound method for determining if groups of eight bands have to be tangled together in a system with inversion symmetry, this consideration of symmetry eigenvalues and commutation relations is beneficial when dealing with three-dimensional space groups for which the platycosm formulation of
the WPVZ bound breaks down. For example, in systems where high-fold rotation leads to an eight-fold double Dirac point, the WPVZ bound calculated through a consideration of flat manifold placement only seems to capture the particular 8-band Dirac feature seen in layer group 45. While the platycosm formulation of the WPVZ bound states that space group 130 has a minimal insulating filling of $8\mathbb{Z}$ and space group 135 a minimal insulating filling of $4\mathbb{Z}$, both crystal systems are very similar in practice and both in practice host essential double Dirac points [224]. The only distinguishing feature between them is that additional Dirac points are present in space group 130 at fillings $\nu \in 4 + 8\mathbb{Z}$, owing to the offset of a screw rotation from the inversion centers. The same set of two-fold nonsymmorphic symmetries lies along the inversion centers in space group 135, and therefore the first part of the criteria for local protection of such Dirac points is not met.

This consideration of two-fold nonsymmorphic symmetries predicts 8-band Dirac features even when the platycosm formulation of the WPVZ bound fails. Space group 73, due to the limitations of the modding procedure as it relates to inversion symmetry, combined with the body-centered geometry of its underlying lattice, is incorrectly predicted to have a minimal insulating filling of $4\mathbb{Z}$ by the platycosm formulation of the WPVZ bound [216]. In a paper released during the final stages of preparing this chapter, WPVZ noted using a similar eigenvalue and commutation algebra consideration that this system, generated only by two-fold nonsymmorphic operations and inversion symmetry, hosts essential eight-band features in the non-interacting limit [217].
Layer Group 33 (Space Group 29)

(a) \[ \mathbf{v}_A = \{ \mathcal{M}_z \mid \frac{1}{2} \}, \{ \mathcal{C}_{2y} \mid 0^\frac{1}{2} \} \]

(b) \[
\begin{array}{cccc}
\bullet & C & \bullet & D \\
\circ & A & \circ & B
\end{array}
\]

(c) \[
\begin{array}{cccc}
\Gamma & M & X & \Gamma \\
-2 & -1 & 0 & 1
\end{array}
\]

(d) \[
\begin{array}{ccc}
S_y, G_z & S_y, G_z & G_z \\
\{ \pm i \} & \{ \pm i \} & \{ \pm i \} \\
\{ +1, +1 \} & \{ +1, -1 \} & \{ +1, +1 \} \\
\{ -1, -1 \} & \{ -1, +1 \} & \{ -1, -1 \}
\end{array}
\]

Figure 6.12: The generators (a), lattice (b), and a typical band structure (c) for layer group 33 pb2_{1}a (space group 29). This is the only layer group which can achieve a WPVZ bound of 8 without inversion symmetry. Bands along ΓY are two-fold-degenerate by the anticommutivity of \( S_y = t_{y/2}c_{2y} \) and \( G_z = t_{x/2}t_{y/2}\mathcal{M}_z \). Bands along \( Y\hat{M} \) are two-fold-degenerate by the combination of \( G_z \) and \( \mathcal{T} \). Even though the layer group only consists of two-fold nonsymmorphic symmetries without inversion, the combination of symmetries is such that eight bands have to be tangled together along \( \Gamma X \) and \( X\hat{M} \). Listing the eigenvalues of \( S_y \) and \( G_z = t_{x/2}\mathcal{M}_z \) (d), the evolution of the two-fold nonsymmorphic eigenvalues for each symmetry \( \lambda_\pm = \pm ie^{\pm ik_x/\sqrt{2}} \) causes bands to form characteristic four-band structures as explained in Ref. 245. Starting at \( \Gamma \), one can choose parameters such that along \( \Gamma X \) there is a gap at half filling with these four-band structures above and below the gap. However, because \( [S_y, G_z] = 0 \) along \( X\hat{M} \), the four-band structures which form along \( X\hat{M} \) preserve the eigenvalue of \( G_z \) (±1 indicated as a dashed or solid line respectively) and exchange new partners with local protection, forming a sort of 8-band “cat’s cradle” structure and filling in the gap at \( \nu = 4 \) with essential Weyl points. Should one tune parameters as to open up a gap along \( X\hat{M} \), the resultant Weyl points at half filling will instead form along \( \Gamma X \).
The WPVZ bound proves most advantageous when considering systems without inversion, In layer group 33 $pba_1$ (space group 29) (Fig. 6.12(a)), there is no inversion symmetry, and so bands can only become two-fold-degenerate by the combination of $T$ and a two-fold nonsymmorphic symmetry (here $G_x = t_x/2t_y/2M_z$ for $\overline{YM}$) or by the anticommutivity of two spatial symmetries along a common line (here $S_y = t_y/2C_{2y}$ and $G_z$ along $\Gamma Y$) (Fig. 6.12(c)). However, neither set of two-fold-degenerate bands contributes to obvious eight-band essential Dirac features, and one might be tempted when just considering symmetry eigenvalues to guess that this layer group is an insulator at $\nu = 4$. However, because this four-site system has $S_y$ and $G_z = t_x/2M_z$, placement is still allowed onto the 1st amphidicosm and WPVZ predict that 8 bands must be tangled together across the 2D BZ. Observing the band structure (Fig. 6.12(c)), there is in fact an essential eight-band, “cat’s cradle-like” Weyl feature present along the path $\Gamma X \cup XM$, with all four essential Weyl points laying along the same line.

These essential Weyl points can be explained by examining the evolution of nonsymmorphic symmetry eigenvalues $\lambda_{\pm} = \pm ie^{ik_x/2}$ (Fig. 6.12(d)). Consider choosing parameters such that along $\Gamma X$ bands are separated into two four-band, hourglass-like structures with a gap at $\nu = 4$. For most layer groups, these four-band structures would be the extent of the essential band-tangling features and the system could remain gapped at $\nu = 4$ across the entire 2D BZ. However, because in layer group 33 $[S_y, G_z] = 0$ along $XM$, the four-band structures which form along $XM$ preserve the eigenvalue of $G_z$ ($\pm 1$ indicated as a dashed or solid line respectively
in Fig. 6.12(d)) and exchange new partners with local protection, forming a sort of 8-band “cat’s cradle” structure and filling in the gap at \( \nu = 4 \) with essential Weyl points. Should one tune parameters as to open up a gap along \( \overline{XM} \), the resultant Weyl points at half filling will instead form along \( \overline{\Gamma X} \).

6.6 Discussion

In this chapter, we have fully characterized the essential nodal semimetallic band features allowed in the layer groups. By using a bound on the minimal insulating filling, derived from the compatibility between symmetry generators of a layer group and embedding the underlying lattice onto a flat compact manifold, we found that there can be layer group semimetals with interlocking groups of 2, 4, or 8 bands which cannot be untangled without lowering the spatial symmetry of the system. This bound was achieved following a procedure by Watanabe, Po, Vishwanath, and Zaletel (WPVZ) in Ref. 216 valid for both interacting and noninteracting systems which, though failing in select cases in three dimensions [27, 217, 224], is complete for all of the space groups which derive from trivial stackings of the wallpaper and layer groups. Within layer groups with minimal insulating fillings of \( 4\mathbb{Z} \), the results of Ref. 245 can be recovered, but one can also find new features, such as a band-inversion-type Dirac semimetal protected by an inversion-center offset. Three layer group systems, specifically layer groups 33, 43, and 45 (space groups 29, 54, and 57, respectively, when stacked) can achieve minimal insulating fillings of \( 8\mathbb{Z} \). Layer
groups 54 and 57 have inversion symmetry, and are therefore Dirac semimetals at fillings $\nu \in 4 + 8\mathbb{Z}$, with their 8-band essential Dirac features owing to the same mechanism of symmetry protection as the line node in SrIrO$_3$ [34]. Layer group 33, however, does not have inversion, and instead has a previously uncharacterized essential eight-band “cat’s cradle” Weyl fermion feature with four essential Weyl points present along a high-symmetry line at fillings $\nu \in 4 + 8\mathbb{Z}$.

In addition to the constraints imposed on the band features of quasi-two-dimensional mono- or few-layer systems, this consideration of compact flat manifold placements, specifically for the strictly two-dimensional wallpaper systems in 6.3.1, also provides restrictions on the allowed band features on the surfaces of three-dimensional systems. For groupings of bands which don’t require a bulk to exist, namely the trivially-connected states of topological crystalline insulators, such as the “hourglass fermions” in Ref. 214, this bound indicates that *symmetry can force, at most, four bands to be tangled together on the surface of a three-dimensional system*. As there are only four wallpaper groups with glide lines, this further constrains the possible topological surface band flows as well. Considering the allowed band features in the wallpaper groups, a combination of symmetry analysis and minimal insulating filling restrictions should allow one to exhaustively deduce all possible “hourglass”-like surface flows permitted in bulk-insulating systems.

Finally, the two-dimensional and quasi-two-dimensional systems characterized in this chapter can provide significant benefits over their three-dimensional counter-
parts. They are considerably easier to visualize and analyze by crystalline symmetry. They are also easier to simulate in tight-binding and density functional theory calculations, allowing for a relatively fast route towards predicting and engineering two-dimensional nodal semimetals, including eight-band structures analogous to those in three dimensions. These systems can also allow experimental access to two-dimensional topological physics. As characterized in Ref. 245, nonsymmetric two-dimensional materials can be pinned by an additional symmetry to the quantum critical point between a trivial and a topological insulator, and therefore one could consider them as parent materials for examining strain-engineered topological phase transitions.

6.7 Chapter Acknowledgments

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Figure 6.13: A 2-torus (a) and two Klein bottles with a common boundary (b). In order to create a shape with the same external arrows as the 2-torus, two Klein bottles have to be placed together, sharing the common twisted boundary. This procedure is the origin of the bold numbers in Figures 6.1 and 6.2. For a four-site unit cell, this decimation factor, \( n_{\text{dec}} = A_{\text{unit}} / A_{\text{dec}} \) where \( A \) is the area of the original and decimated unit cells respectively, gives the minimal insulating filling constraint \( \nu \in 2n_{\text{dec}}\mathbb{Z} \).

6.8 Appendix

6.8.1 Further Notes on and Examples of Decimations and Flat-Manifold Placement

In this appendix, we visually detail the decimation procedure from Figure 6.3 in layered two-dimensional systems.

For layered two-dimensional systems, the consideration of minimal insulating filling is completely captured by the number of fixed-point-free decimations of a four-site unit cell. One can consider this unit cell as being the final one before the boundary in both the \( x \) and \( y \) (in-plane) directions. As one row of atoms is chopped
off and the coordinate-axis boundary condition twisted, this unit cell is decimated by modding out the nonsymmorphic symmetry which related the atoms remaining to those removed by decimation. We can consider for any manifold a decimation factor:

\[
  n_{\text{dec}} = \frac{A_{\text{unit}}}{A_{\text{dec}}}
\]  

(6.8.1)

which measures the ratio of the areas of the original to the decimated unit cell. This factor is precisely the bold numbers indicated in Figures 6.1 and 6.2, which could also be expressed as the number of times a manifold would have to be repeated with a common boundary in order to create a supercell with the same external boundary as the 2-torus in wallpaper systems, or the 3-torus in general layer group systems (Figure 6.13). For a four-site unit cell in two dimensions, the insulating fillings, absent any additional band inversions, are therefore:

\[
  \nu \in 2n_{\text{dec}}\mathbb{Z}.
\]  

(6.8.2)

A central part of this procedure is the restriction that we only utilized fixed-point-free decimations. As emphasized in the main text, *multiple decimations by two-fold operations are only allowed if the product of those operations is itself also an inherently nonsymmorphic operation* [89, 216].

243
Figure 6.14: A demonstration of the decimation procedure for two layer groups with multiple nonsymmorphic symmetries. The minimal insulating filling is proportional to the ratio of the sizes of the maximally decimated unit cell to that of the original, with special consideration given to avoid decimations which introduce fixed points. Layer group 21 (space group 18) (a) is generated by two perpendicular screws: $S_{x/y} = t_{x/y}/2C_{2x/y}$. One could choose to mod out $S_x$ first, reducing the area of the unit cell by half and placing the system onto the dicosm. However, further decimation by $S_y$ would then be disallowed, because $S_xS_y \sim t_{x/2}t_{y/2}(C_{2z})$, which is an inherently symmorphic operation ($C_{2z}$ about the center of the unit cell). Therefore, choosing either screw, the maximal decimation of layer group 21 gives $n_{\text{dec}} = 2$ and placement onto the dicosm, with a minimal insulating filling of $\nu \in 4\mathbb{Z}$. Conversely, layer group 33 (space group 29) (b) is generated by $S_y$ and $G_z = t_{x/2}M_z$. Modding out $G_z$ first removes the right half of the unit cell and places the system onto the 1st amphicosm. However, this is not the maximal decimation, as the product $S_yG_z \sim t_{x/2}(t_{y/2}M_z)$, which is an inherently nonsymmorphic operation. Therefore, layer group 33 admits an additional decimation by $S_y$ onto the 1st amphidicosm, resulting in $n_{\text{dec}} = 4$ and a minimal insulating filling of $\nu \in 8\mathbb{Z}$. 
Figure 6.14 illustrates two examples of layer groups with multiple nonsymmmorphic group elements. Layer group 21 (space group 18) (Fig. 6.14(a)) is generated by two perpendicular screws: $S_{x/y} = t_{x/y/2}C_{2x/y}$. One could choose to mod out $S_x$ first, reducing the area of the unit cell by half and placing the system onto the dicosm. However, further decimation by $S_y$ would then be disallowed, because $S_xS_y \sim t_{x/2}t_{y/2}(C_{2z})$, which is an inherently symmorphic operation ($C_{2Z}$ about the center of the unit cell). Therefore, choosing either screw, the maximal decimation of layer group 21 gives $n_{\text{dec}} = 2$ and placement onto the dicosm, with a minimal insulating filling of $\nu \in 4\mathbb{Z}$. Conversely, layer group 33 (space group 29) (Fig. 6.14(b)) is generated by $S_y$ and $G_z = t_{x/2}M_{z}$. Modding out $G_z$ first removes the right half of the unit cell and places the system onto the 1st amphicosm. However, this is not the maximal decimation, as the product $S_yG_z \sim t_{x/2}(t_{y/2}M_{z})$, which is an inherently nonsymmmorphic operation. Therefore, layer group 33 admits an additional decimation by $S_y$ onto the 1st amphidicosm, resulting in $n_{\text{dec}} = 4$ and a minimal insulating filling of $\nu \in 8\mathbb{Z}$.

6.8.2 Tight-Binding Models

In this appendix, we list the tight-binding Hamiltonians for the example layer groups selected for this chapter (Figs. 6.6-6.12).

We begin by considering a four-site rectangular unit cell in two dimensions (Fig. 6.5). Initially, each site has spherical symmetry such that this high-symmetry
system can be considered a relabeling of a rectangular one-site unit cell with all of
the symmetries of the underlying Bravais lattice. Repeating the procedure from 6.5,
we designate Pauli matrices for the sublattice degrees of freedom, with $\tau^x$ indicating
s-orbital-like hopping between the A and B (and C and D) sites and $\mu^x$ indicating
s-orbital-like hopping between the A and C sites (and B and D) such that $\tau^x\mu^x$
indicates s-like-hopping between A and D sites (and B and C). Each site is given
an additional spin degree of freedom $\sigma$ such that our overall model has eight bands.

We can, in this high-symmetry limit, first write down all of the first- and second-
nearest-neighbor s-orbital-like hopping terms:

$$
\mathcal{H}_0 = t_x \cos \left( \frac{k_x}{2} \right) \tau^x + t_y \cos \left( \frac{k_y}{2} \right) \mu^x \\
+ t_2 \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) \tau^x \mu^x 
$$

(6.8.3)

where the lattice spacing $a_{x/y}$ has been set to 1. From there, terms can be
added to reduce the symmetry of the system into a particular layer group and lift
many of the degeneracies. For a particular layer group $LG$, we consider the set of
all symmetry-allowed first- and second-nearest-neighbor hoppings (other than the
existing s-like ones) to be a potential $V_{LG}$ such that overall $\mathcal{H}_{LG} = \mathcal{H}_0 + V_{LG}$. We find
that using all of the terms up to second-nearest-neighbor interactions produces layer-
group-specific band structures (though occasionally allows for an artificial chiral
symmetry, which could be broken by introducing symmetry-allowed third-nearest-neighbor terms).

For each layer group, the allowed terms $V_{LG}$ can be determined by considering how the group generators transform a generic Hamiltonian $\mathcal{H}(k_x, k_y)$ and finding all physical hopping terms invariant under that transformation. In practice, the form of the representation of each group generator in the sublattice and Bloch space is that of the representation at $\Gamma$ multiplied by an operation on $\vec{k}$. Additionally, all systems are considered to be time-reversal symmetric with $T = i\sigma^y K \otimes (\vec{k} \to -\vec{k})$ such that $T^2 = -1$.

In the following subsections, we detail the group generators and $V_{LG}$ for each of the example systems in the text. All generators are defined from the common origin of site A. In order, the generators are described by the name of the generator, the generator as operations defined from site A, and the form of the representation of the operator for our eight-band $\mathcal{H}(\vec{k})$. Similar terms are grouped under the same constants for simplicity, though this is not explicitly required by symmetry. Values of the constants used for band plots have been noted after each $V_{LG}$.

6.8.2.1 Layer Group 37

Layer group 37, $pmmm$ (space group 47) has a WPVZ bound of 2 and the following generators:
\[ M_{\hat{x}} = t_{x/2} M_{\hat{x}} = \tau^x \sigma^z \otimes (k_x \rightarrow -k_x) \]
\[ M_{\hat{y}} = t_{y/2} M_{\hat{y}} = \mu^x \sigma^y \otimes (k_y \rightarrow -k_y) \]
\[ M_{\hat{z}} = M_{\hat{z}} = \sigma^z. \quad (6.8.4) \]

This results in the following allowed first- and second-nearest-neighbor hopping terms:

\[ V_{37} = \cos \left( \frac{k_x}{2} \right) \left[ v_{r1x} \tau^y \mu^z \sigma^z \right] \]
\[ + \sin \left( \frac{k_x}{2} \right) \left[ v_{p1x} \tau^y + v_{s1x} \tau^x \mu^z \sigma^z \right] \]
\[ + \cos \left( \frac{k_y}{2} \right) \left[ v_{r1y} \tau^x \mu^z \sigma^z \right] \]
\[ + \sin \left( \frac{k_y}{2} \right) \left[ v_{p1y} \mu^y + v_{s1y} \tau^z \mu^x \sigma^z \right] \]
\[ + \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) \left[ v_{p2} \tau^y \mu^x \right] \]
\[ + \cos \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) \left[ v_{p2} \tau^x \mu^y \right] \]
\[ + \sin \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) \left[ v_{p2} \tau^y \mu^y \right]. \quad (6.8.5) \]

For the bands in Fig. 6.6(c),
\[ t_x = 1.0, \quad t_y = 1.25, \quad t_2 = 0.4, \quad v_{r1x} = 0.3, \]
\[ v_{plx} = 0.35, \quad v_{s1x} = -0.65, \quad v_{r1y} = 0.45, \quad v_{ply} = 0.65 \]
\[ v_{v1y} = -0.8, \quad v_{p2} = -0.2. \quad (6.8.6) \]

**6.8.2.2 Layer Group 23**

Layer group 23, \textit{pmm2} (space group 25), has a WPVZ bound of 2. It is the result of breaking \( M\hat{z} \) in layer group 37, leading to the following generators:

\[ M_{\hat{x}} = t_{x/2}M_{\hat{x}} = \tau^x \sigma^x \otimes (k_x \rightarrow -k_x) \]
\[ M_{\hat{y}} = t_{y/2}M_{\hat{y}} = \mu^x \sigma^y \otimes (k_y \rightarrow -k_y). \quad (6.8.7) \]

The allowed terms in layer group 23 can be therefore considered as those allowed for layer group 37, plus new terms which don’t commute with \( \sigma^z \):
\[ V_{23} = V_{37} \]
\[ + \cos \left( \frac{k_x}{2} \right) [u_{r1x} \tau^{y} \sigma^{y}] + \sin \left( \frac{k_x}{2} \right) [v_{s1x} \tau^{x} \sigma^{y}] \]
\[ + \cos \left( \frac{k_y}{2} \right) [v_{r1y} \mu^{y} \sigma^{x}] + \sin \left( \frac{k_y}{2} \right) [v_{s1y} \mu^{x} \sigma^{x}] \]
\[ + \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{r2} (\tau^{x} \mu^{y} \sigma^{x} + \tau^{y} \mu^{x} \sigma^{y})] \]
\[ + \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{s2} (\tau^{x} \mu^{x} \sigma^{x} + \tau^{y} \mu^{y} \sigma^{x})] \]
\[ + \cos \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{s2} (\tau^{x} \mu^{x} \sigma^{x} + \tau^{y} \mu^{y} \sigma^{y})] \]
\[ + \sin \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{r2} (\tau^{x} \mu^{y} \sigma^{y} + \tau^{y} \mu^{x} \sigma^{x})] . \]

(6.8.8)

For the bands in Fig. 6.7(c),

\[ t_x = 1.0, \ t_y = 1.25, \ t_2 = 0.1, \ v_{r1x} = 0.3, \]
\[ v_{plx} = 0.35, \ v_{s1x} = -0.65, \ v_{r1y} = 0.45, \ v_{p1y} = 0.65 \]
\[ v_{es1y} = 0.7, \ v_{p2} = -0.2, \ v_{s2} = -0.35, \ v_{r2} = 0.3. \]

(6.8.9)

For the bands in Fig. 6.7(d),
\[ t_x = 1.0, \quad t_y = 1.25, \quad t_2 = 0.9, \quad v_{r_{1x}} = 0.3, \]

\[ v_{p_{1x}} = 0.35, \quad v_{s_{1x}} = -0.65, \quad v_{r_{1y}} = 0.45, \quad v_{p_{1y}} = 0.65 \]

\[ v_{v_{s1y}} = 0.7, \quad v_{p2} = -0.9, \quad v_{s2} = -0.35, \quad v_{r2} = 0.1. \quad (6.8.10) \]

### 6.8.2.3 Layer Group 44

Layer group 44, \textit{pbam} (space group 55) has a WPVZ bound of 4 and the following generators:

\[ S_x = \frac{t_x}{2} C_{2x} = \tau^x \sigma^x \otimes (k_y \rightarrow -k_y) \]

\[ S_y = \frac{t_y}{2} C_{2y} = \mu^x \sigma^y \otimes (k_x \rightarrow -k_x) \]

\[ M_z = M_{\hat{z}} = \sigma^z. \quad (6.8.11) \]

This results in the following allowed first- and second-nearest-neighbor hopping terms:
\[ V_{44} = \cos \left( \frac{k_x}{2} \right) [v_{r1x} \tau^y \mu^z \sigma^z] + \cos \left( \frac{k_y}{2} \right) [v_{r1y} \tau^z \mu^y \sigma^z] \]
\[ + \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{r2} \tau^x \mu^y] \]
\[ + \cos \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{r2} \tau^y \mu^x] \]
\[ + \sin \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{r2} \tau^y \mu^y]. \] (6.8.12)

For the bands in Fig. 6.8(c),

\[ t_x = 1.0, \quad t_y = 1.55, \quad t_2 = 0.4, \quad v_{r1x} = 0.3, \]
\[ v_{vr1y} = 0.6, \quad v_{r2} = 0.2. \] (6.8.13)

**6.8.2.4 Layer Group 21**

Layer group 21, \( p2_12_12 \) (space group 18), has a WPVZ bound of 4. It is the result of breaking \( M \hat{z} \) in layer group 44, leading to the following generators:

\[ S_x = t_{x/2} C_{2x} = \tau^x \sigma^x \otimes (k_y \rightarrow -k_y) \]
\[ S_y = t_{y/2} C_{2y} = \mu^x \sigma^y \otimes (k_x \rightarrow -k_x). \] (6.8.14)
The allowed terms in layer group 21 can be therefore considered as those allowed for layer group 44, plus new terms which don’t commute with $\sigma^z$:

\[
V_{21} = V_{44} + \cos \left( \frac{k_x}{2} \right) [v_{r1x} (\tau^y \sigma^y + \tau^y \mu^z \sigma^z)] \\
+ \sin \left( \frac{k_x}{2} \right) [v_{s1x} \tau^x \sigma^x] \\
+ \cos \left( \frac{k_y}{2} \right) [v_{r1y} (\mu^y \sigma^x + \tau^z \mu^y \sigma^z)] \\
+ \sin \left( \frac{k_y}{2} \right) [v_{s1y} \mu^x \sigma^y] \\
+ \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{r2} (\tau^x \mu^y \sigma^x + \tau^y \mu^x \sigma^z)] \\
+ \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{s2} (\tau^x \mu^z \sigma^x + \tau^y \mu^y \sigma^y)] \\
+ \cos \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{s2} (\tau^x \mu^y \sigma^x + \tau^y \mu^x \sigma^z)] \\
+ \sin \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{r2} (\tau^x \mu^x \sigma^y + \tau^y \mu^y \sigma^z)].
\]

(6.8.15)

For the bands in Fig. 6.9(c),
\[ t_x = 1.0, \ t_y = 1.55, \ t_2 = 0.4, \ v_{r1x} = 0.3, \]
\[ v_{s1x} = 0.65, \ v_{vr1y} = 0.6, \ v_{s1y} = 0.85, \]
\[ v_{r2} = 0.6, \ v_{s2} = 0.7. \] (6.8.16)

6.8.2.5 Layer Group 17

Layer group 17, \( p\overline{2}1/b11 \) (space group 14) has a WPVZ bound of 4 and the following generators:

\[ I = t_y/2I = \mu^x \otimes (\vec{k} \rightarrow -\vec{k}) \]
\[ G_y = t_x/2M_{\hat{y}} = \tau^x \sigma^y \otimes (k_y \rightarrow -k_y). \] (6.8.17)

This results in the following allowed first- and second-nearest-neighbor hopping terms:
\[ V_{17} = \cos \left( \frac{k_x}{2} \right) [v_{r1x} \tau^y \sigma^x] + \sin \left( \frac{k_x}{2} \right) [v_{s1x} \tau^x \mu^z \sigma^y] \]

\[ + \sin \left( \frac{k_y}{2} \right) [v_{p1y} \tau^z \mu^y] \]

\[ + \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{p2x} \tau^x \mu^y \sigma^x] \]

\[ + \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{p2x} \tau^x \mu^y \sigma^y + v_{s2} \tau^y \mu^y \sigma^x] \]

\[ + \cos \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{s2} \tau^y \mu^y \sigma^y] \]

\[ + \sin \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v_{r2} \tau^y \mu^x \sigma^y] \quad (6.8.18) \]

noting that additional terms are also allowed due to this system’s invariance under \( \sigma^x \leftrightarrow \sigma^z \).

For the bands in Fig. 6.10(c),

\[ t_x = 1.0, \ t_y = 1.14, \ t_2 = 0.4, \ v_{r1x} = 0.3, \]
\[ v_{s1x} = 0.65, \ v_{p1y} = 0.8, \ v_{r2} = 0.25, \]
\[ v_{p2} = 0.2, \ v_{s2} = 0.45. \quad (6.8.19) \]

For the bands in Fig. 6.10(d),

255
\begin{align*}
t_x &= 1.0, \quad t_y = 1.14, \quad t_2 = 0.4, \quad v_{r1x} = 0.3, \\
v_{s1x} &= 0.65, \quad v_{vp1y} = 0.2, \quad v_{y2} = 0.25, \\
v_{p2} &= 0.2, \quad v_{s2} = 0.45. \quad (6.8.20)
\end{align*}

\subsection*{6.8.2.6 Layer Group 45}

Layer group 45, \textit{pbma} (space group 57) has a WPVZ bound of 8 and the following generators:

\begin{align*}
G_z &= t_{x/2}M_{z} = \tau^x \sigma^z \\
S_y &= t_{x/2}t_{y/2}C_{2y} = \tau^x \mu^x \sigma^y \otimes (k_x \rightarrow -k_x) \\
\mathcal{I} &= t_{x/2}t_{y/2}\mathcal{I} = \tau^x \mu^x \otimes (\mathbf{k} \rightarrow -\mathbf{k}). \quad (6.8.21)
\end{align*}

This results in the following allowed first- and second-nearest-neighbor hopping terms:
\[ V_{45} = \cos \left( \frac{k_x}{2} \right) [v_{r1x} \tau^y \mu^z \sigma^y] + \cos \left( \frac{k_y}{2} \right) [v_{r1y} \tau^z \mu^y \sigma^y] \]

\[ + \sin \left( \frac{k_y}{2} \right) [v_{s1y} \tau^z \mu^x \sigma^x] \]

\[ + \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{p2} \tau^x \mu^y]. \]  

(6.8.22)

For the bands in Fig. 6.11(c),

\[ t_x = 1.0, \quad t_y = 1.25, \quad t_2 = 0.4, \quad v_{r1x} = -0.3, \]

\[ v_{r1y} = 0.45, \quad v_{s1y} = 0.8, \quad v_{p2} = -0.2. \]  

(6.8.23)

6.8.2.7 Layer Group 33

Layer group 33, \( pb2_1a \) (space group 29) has a WPVZ bound of 8 and the following generators:

\[ G_z = t_{x/2} M_z = \tau^x \sigma^z \]

\[ S_y = t_{y/2} C_{2y} = \mu^x \sigma^y \otimes (k_x \rightarrow -k_x). \]  

(6.8.24)
\[ V_{33} = \cos\left(\frac{k_x}{2}\right) [v_{r1x} \tau^y \mu^z \sigma^x] + \sin\left(\frac{k_x}{2}\right) [v_{s1x} \tau^x \sigma^z] \]
\[ + \cos\left(\frac{k_y}{2}\right) [v_{r1y} (\tau^z \mu^y \sigma^x + \mu^y \sigma^z)] \]
\[ + \sin\left(\frac{k_y}{2}\right) [v_{s1y} \tau^z \mu^x \sigma^y] \]
\[ + \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{k_y}{2}\right) [v_{r2} (\tau^y \mu^x \sigma^y + \tau^x \mu^y \sigma^z)] \]
\[ + \sin\left(\frac{k_x}{2}\right) \cos\left(\frac{k_y}{2}\right) \times \]
\[ [v_{p2} \tau^x \mu^y + v_{s2} (\tau^y \mu^y \sigma^x + \tau^x \mu^x \sigma^z)] \]
\[ + \cos\left(\frac{k_x}{2}\right) \sin\left(\frac{k_y}{2}\right) [v_{s2} \tau^y \mu^y \sigma^x] \]
\[ + \sin\left(\frac{k_x}{2}\right) \sin\left(\frac{k_y}{2}\right) [v_{r2} \tau^y \mu^y \sigma^x] . \]  
(6.8.25)

For the bands in Fig. 6.12(c),

\[ t_x = 1.0, \ t_y = 1.25, \ t_z = 0.4, \ v_{r1x} = -0.3, \]
\[ v_{s1x} = 0.3, \ v_{r1y} = 0.45, \ v_{s1y} = 0.8, \]
\[ v_{r2} = 0.25, \ v_{p2} = -0.2, \ v_{s2} = 0.45. \]  
(6.8.26)
6.8.3 List of Filling Conditions for the 80 Layer Groups

In this appendix, we list the 80 layer groups as sorted by their allowed platycosm placements. For each layer group, we cite the equivalent space group for a three-dimensional stack of that system [87].

The 17 layer groups which could additionally describe the boundary of a three-dimensional object also comprise the wallpaper groups and are denoted with (w). These groups contain no operations which would exchange the interior and exterior of such a three-dimensional object, and therefore (if $\hat{z}$ is the layer stacking direction or surface normal) are disallowed from having $P$, $M_{\hat{z}}$, or $C_{2x/y}$, as well as any of those operations followed by a fractional lattice translation.

Layer groups without nonsymmorphic symmetries are only allowed placement onto the torocosm, or 3-torus, and have no insulating filling constraints besides $\nu \in 2\mathbb{Z}$ by Kramers’ theorem.

Layer groups with two-fold screws and no glide mirrors can be decimated and placed onto the two-sided dicosm, which results in insulating fillings of $\nu \in 4\mathbb{Z}$ absent any additional band inversions with locally-protected crossings (otherwise stated as the “minimal-insulating filling”).

Layer groups with glide mirrors and no two-fold screws can be decimated and placed onto the one-sided 1st amphicosm, which results in a minimal insulating
### 3-Torus \((43 \text{ Layer Groups})\)

<table>
<thead>
<tr>
<th>Layer Group (\nu \in 2\mathbb{Z})</th>
<th>Space Group</th>
<th>Layer Group (\nu \in 2\mathbb{Z})</th>
<th>Space Group</th>
</tr>
</thead>
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<td>1 (w)</td>
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</tr>
<tr>
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</tr>
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<td>49 (w)</td>
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<tr>
<td>51</td>
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</tr>
</tbody>
</table>

Table 6.1: Layer groups allowed placement onto the 3-torus, with minimal insulating fillings of \(\nu \in 2\mathbb{Z}\).

### Only Dicosm \((6 \text{ Layer Groups})\)

<table>
<thead>
<tr>
<th>Layer Group (\nu \in 4\mathbb{Z})</th>
<th>Space Group</th>
<th>Layer Group (\nu \in 4\mathbb{Z})</th>
<th>Space Group</th>
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</table>

Table 6.2: Layer groups allowed placement onto only the dicosm, with minimal insulating fillings of \(\nu \in 4\mathbb{Z}\).
Table 6.3: Layer groups allowed placement onto only the 1st amphicosm, with minimal insulating fillings of $\nu \in 4\mathbb{Z}$.

Layer groups with both glide mirrors and two-fold screws require more careful examination. As part of the procedure for decimation from 6.3 and Appendix 6.8.1, all combinations of perpendicular nonsymmorphic symmetries must be examined to determine if further decimation is allowed from the dicosm or 1st amphicosm into the 1st amphidicosm. *For the layer groups, that decimation is in practice only allowed for systems with four or more sites per unit cell and any $z$-axis rotation of $S_y = t_{y/2}C_{2y}$ and $G_z = t_{x/2}M_z$.*

Absent these conditions, for layer groups with both glide mirrors and screws, frequently the case in those with inversion symmetry, one could choose to mod out using *either* the glide or the two-fold screw, allowing placement onto either the dicosm or the 1st amphidicosm. For both cases, the filling restrictions are the same: an insulator can only occur at fillings of $\nu \in 4\mathbb{Z}$.
Table 6.4: Layer groups allowed placement onto either the dicosm of the 1st amphicosm, with minimal insulating fillings of $\nu \in 4\mathbb{Z}$.

<table>
<thead>
<tr>
<th>Layer Group</th>
<th>Space Group</th>
<th>Layer Group</th>
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<tr>
<td>41</td>
<td>51</td>
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</tbody>
</table>

Table 6.5: Layer groups allowed placement onto either the 1st amphidicosm, with minimal insulating fillings of $\nu \in 8\mathbb{Z}$.

<table>
<thead>
<tr>
<th>Layer Group</th>
<th>Space Group</th>
<th>Layer Group</th>
<th>Space Group</th>
</tr>
</thead>
<tbody>
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<td>33</td>
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</tr>
<tr>
<td>43</td>
<td>54</td>
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</tbody>
</table>

Finally, these conditions for further decimation onto to the one-sided 1st amphidicosm are, in fact, only satisfied by 3 layer groups. For these groups, eight bands have to be tangled together, and therefore these 3 layer groups have minimal insulating fillings of $\nu \in 8\mathbb{Z}$.
Chapter 7

Topological Dirac Insulators

7.1 Abstract

Recent interest in the relationship between bulk topology and surface crystalline symmetries has fueled the development and discovery of such materials as mirror topological crystalline insulators and nonsymmorphic hourglass fermion insulators. In fact, there exists only a very limited set of possible surface crystal symmetries, captured by the 17 “wallpaper groups.” Here, we show that all possible crystalline insulators, symmorphic and nonsymmorphic, can be exhaustively characterized by a consideration of these wallpaper groups. In particular, the two wallpaper groups with multiple glide lines, \( pgg \) and \( p4g \), allow for a new topological insulating phase, whose surface spectrum consists of only a single, \( \textit{four-fold degenerate} \), true Dirac
fermion. Like the surface state of a conventional topological insulator, this surface Dirac fermion provides a theoretical exception to a fermion doubling theorem. Unlike the surface state of a conventional topological insulator, it can be gapped into topologically distinct surface regions while keeping time-reversal symmetry, allowing for networks of topological surface quantum spin Hall domain walls. For orthorhombic space groups with two perpendicular glides, we catalog all possible bulk topological phases by a consideration of the allowed non-Abelian Wilson loop connectivities, and provide topological invariants to distinguish them. Finally, we show how in a particular limit of these systems, the crystalline phases reduce to copies of the Su-Schrieffer-Heeger model, and we present a simple tight-binding model which captures all allowed phases. *This chapter is reproduced from a paper in preparation by Benjamin J. Wieder*, Barry Bradlyn*, Zhijun Wang*, Jennifer Cano*, Youngkuk Kim, Hyeong-Seok D. Kim, A. M. Rappe, C. L. Kane, and B. Andrei Bernevig.*

### 7.2 Introduction

Topological phases stabilized by crystal symmetries have already proven to be both a theoretically and an experimentally rich class of systems. The first class of these proposed materials, mirror topological crystalline insulators (TCIs), host surface fermions protected by the projection of a bulk mirror symmetry to a particular surface[60, 201]. They have been observed in SnTe[94, 196] and related
compounds[50, 234]. Recent efforts to expand this analysis to systems with nonsymmetric surface glide mirrors – operations composed of a mirror and a half-lattice translation – have yielded additional exotic free fermion topological phases, such as those with so-called surface gapless “hourglass fermions,” and the glide spin-hall effect[9, 37, 130, 185, 214]. The theoretical proposal of Refs. 9, 214 has recently also been experimentally confirmed [138].

In addition, topological insulators (TIs) – crystalline or otherwise – provide exceptions to fermion doubling theorems. These theorems provide deep bounds on phenomena in condensed matter physics. The simplest doubling theorem states that in 2D, a single Kramers pair protected by time-reversal symmetry must always have a partner elsewhere in the Brillouin Zone (BZ), otherwise the Berry phase of a loop around it suffers from ambiguity[14, 158]. The discovery of the topological insulator provided the first exception to this theorem in 3D: its 2D Kramers pairs are allowed to be isolated on a single 2D surface, as they are connected to a 3D bulk and have partners on the opposite surface[61, 93, 148, 231, 258].

Higher-fold degenerate bulk fermions, such as Dirac points, which are stabilized by crystal symmetry, may come with their own fermion doubling theorems[24, 27, 32, 38, 135, 191, 224, 244]. As noted in Ref. 245, and shown in more detail in the supplement, a single four-fold-degenerate Dirac fermion cannot be stabilized by crystal symmetries as the only nodal feature at any filling of a self-contained 2D crystal. Rather, it must always have a partner or accompanying hourglass Weyl
points. This is because a single Dirac point in 2D represents the quantum critical point (QCP) separating a trivial insulator (NI) from a topological insulator. Such a Dirac point cannot be protected by symmetry because otherwise the NI and the TI phases would be equivalent under that symmetry. In this chapter, we report a new class of symmetry-protected topological materials which, like the topological insulator before it, circumvents this restriction by placing a single, stable Dirac point on the surface of a 3D material.

To realize this dream, we crucially require the surface enforcement of multiple non-symmorphic crystal symmetries. Until now, most attention has been paid to crystal systems with surfaces that preserve only a single glide mirror. However, two of the 17 two-dimensional surface symmetry groups, called wallpaper groups, host two intersecting glide lines [44]. As we show in the supplement, the algebra of the two glides requires that bands appear with four-fold degeneracy at a single time reversal invariant momentum (TRIM).

In this work, we study the non-interacting topological phases allowed in bulk crystals with surfaces invariant under the symmetries of these two wallpaper groups, \( pgg \) and \( p4g \). We show that, in addition to generalizations of the hourglass fermions introduced in Ref. [214], they host a novel topological phase characterized by a single, symmetry-enforced four-fold Dirac surface fermion, i.e., with twice the degeneracy of a traditional topological insulator surface state. This 2D Dirac fermion is symmetry-pinned to the QCP between a TI and an NI, allowing for controllable
topological phase transitions under glide-breaking strain.

We classify the allowed topological phases for orthorhombic crystals with two perpendicular glides that are preserved on a single surface by considering the possible connectivities of the non-Abelian Wilson loop eigenvalues[7, 9, 64, 180, 187, 194, 246]. We demonstrate that these systems can host three classes of topological phases: an hourglass phase with broken $C_4z$ symmetry, the novel topological Dirac insulating phase mentioned above, and a previously uncharacterized “double-glide spin hall” phase. We present simple topological invariants to distinguish these phases which could be used to find material realizations.

We conclude with a discussion of the physics of a single surface four-fold Dirac point and its unique promise for strain-engineering gapped surface phases and topologically-protected 1D surface domain walls. In the supplemental material, we show how these crystalline phases reduce in a particular limit to copies of the Su-Schrieffer-Heeger Model (SSH), and we provide a simple tight binding model which can be tuned between all allowed phases.

7.3 Wallpaper Groups $pgg$ and $p4g$

The surface of a crystal is itself a lower-dimensional crystal, which preserves a subset of the bulk crystal symmetries. Despite the myriad symmetry combinations in the 230 3D bulk space groups, all 2D surfaces are geometrically constrained to exist in
Figure 7.1: Unit cells and Brillouin Zone (BZ) for two-site realizations of wallpaper groups $pgg$ and $p4g$, the only two wallpaper groups with multiple nonsymmorphic symmetries. The A and B sites are characterized by $T$-symmetric internal degrees of freedom (blue arrows) that are transformed under crystal symmetry operations. Physically, these could correspond to properties which transform as vectors, such as atom displacements or local electric dipole moments. Glide lines (green) exchange the sublattices. In $p4g$, there is an extra $C_4$ symmetry ($\otimes$) about the surface normal with axes located on the sites. The combination of this $C_4$ and the glides produces additional diagonal symmorphic mirror lines (red) in $p4g$. In the BZ of $p4g$, $C_4$ relates $\bar{Y}$ to $\bar{X}$.

one of the 17 wallpaper groups.

The set of wallpaper symmetry operations is restricted to those which preserve the surface normal vector: rotations about that vector and in-plane mirror or glide lines. The majority of crystal surfaces that have symmetries beyond lattice translations are symmetric under rotation and/or symmorphic mirror operators. Crystals with these surfaces may host quantum spin Hall (QSH) phases and rotational variations of the mirror TCI phases, which exhibit two-fold degenerate free fermions appearing along high-symmetry surface lines[50, 94, 196, 234].

For the four wallpaper groups with nonsymmorphic glide lines ($pg$, $pmg$, $pgg$, and $p4g$), this picture is significantly enriched. Even in 2D, glide symmetries require that groups of four or more bands intersect, an effect which frequently manifests itself in hourglass-like band structures [216, 221, 245]. For the wallpaper groups
with only a single glide line, \( pg \) and \( pmg \), surface bands can be connected in a topologically-nontrivial pattern of interlocking hourglasses, resulting in two-fold degenerate surface fermions along glide lines \[214\]. However, for the remaining two wallpaper groups with multiple orthogonal glide lines, \( pgg \) and \( p4g \), higher-degenerate surface fermions are allowed.

Consider a \( z \)-normal surface with glides \( g_{x,y} \equiv \{ M_{x,y} | \frac{1}{2} \frac{1}{2} 0 \} \) i.e., a mirror reflection through the designated axis, followed by a translation of half a lattice vector in the \( \hat{x} \) and \( \hat{y} \) directions (Fig. 7.1). When spin-orbit coupling is present, \( g_{x,y}^2 = -e^{i k_{x,y}} \). At the corner point, \( M (k_x = k_y = \pi) \), \( g_x^2 = g_y^2 = +1 \), and \( \{ g_x, g_y \} = 0 \). As shown in the supplement, when combined with time-reversal, which satisfies \( T^2 = -1 \), this symmetry algebra requires that all states at \( M \) are four-fold degenerate. Furthermore, wallpaper groups with two glides are the only surface groups that admit this algebra, and therefore the only surface groups that can host protected four-fold degeneracies. Examination of symmetry-allowed terms in the supplemental material reveals that four-fold points in these wallpaper groups will be linearly-dispersing, rendering them true surface Dirac fermions.

For bulk insulators, the allowed glide-preserving bulk topologies and, consequently, the \( z \)-normal surface states, can be determined without imposing a surface by classifying the allowed connectivities of the \( z \)-projection Wilson loop holonomy
Figure 7.2: The eight topologically distinct Wilson band connectivities for bulk insulators with crystal surfaces which preserve two orthogonal glide lines. Each band structure is labeled by its two $\mathbb{Z}_4$ indices, $(\chi_x, \chi_y)$, subject to the constraint that $\chi_x - \chi_y = 0 \mod 2$. Under the imposition of $C_4$ symmetry in wallpaper group $p4g$, connectivities are excluded for which $\chi_x \neq \chi_y$. Solid black (dashed blue) lines in the regions $\bar{X}M$ and $\bar{Γ}Y$ indicate bands with $g_x$ eigenvalue $\pm ie^{ik_y/2}$, while the solid (dashed) lines in the regions $Y\bar{M}$ and $Γ\bar{X}$ indicate bands with $g_y$ eigenvalue $\pm ie^{ik_x/2}$. When inversion symmetry is present, the spectra will be particle-hole symmetric. Bands along $XMY$ are doubly-degenerate and meet at $\bar{M}$ in a four-fold degenerate point, and bands along $YΓX$ display either the hourglass (left column) or “double-glide spin Hall” (right column) flows. The (2,0) and (0,2) phases are relatives of the hourglass topologies proposed in Refs. 9, 214. The novel (2,2) topological Dirac insulating phase can host a surface state consisting of a single, four-fold degenerate Dirac fermion.
matrix[7, 9, 57], a bulk quantity defined by:

\[ \mathcal{W}_{(k_x,k_y,k_z)} \equiv V \left( P e^{i \int_{k_z=0}^{k_z+2\pi} dk_z A_z(k_x,k_y,k_z)} \right) \], \tag{7.3.1} \]

where \( P \) indicates that the integral is path-ordered, \( A_z(k)_{ij} \equiv i \langle u^i(k) | \partial_{k_z} u^j(k) \rangle \) is the matrix-valued Berry connection, and \( V \) is a gauge transformation relating the wavefunctions in adjacent BZs. The rows and columns of \( \mathcal{W} \) correspond to filled bands, and \( |u_{j,k}⟩ \) is an occupied eigenstate at momentum \( k \) with band index \( j \).

The eigenvalues of \( \mathcal{W} \) are gauge invariant and of the form \( e^{i \theta(k_x,k_y)} \). As detailed in the supplement, the Wilson bands inherit the symmetries of the \( z \)-normal wallpaper group and therefore, must also exhibit the required degeneracy multiplets of wallpaper groups \( pgg \) and \( p4g \). In particular, both surface and Wilson bands are two-fold degenerate along \( \bar{X} \bar{M} \) (\( \bar{Y} \bar{M} \)) by the combination of time-reversal and \( g_y \) \( (g_x) \) and meet linearly in four-fold degeneracies at \( \bar{M} \).

By generalizing the \( Z_4 \) invariant defined in Ref. 185 for single-glide wallpaper groups[10, 11], we define topological invariants for double-glide systems using the (001)-surface Wilson loop eigenvalues. For each glide, we define a quantized \( Z_4 \) invariant on a path of three of the four exterior lines of the surface BZ. For \( g_y \) in a surface BZ in wallpaper group \( pgg \), the invariant \( \chi_y \) is obtained by integrating the
Wilson phases, $\theta_j(k_x, k_y)$, along the path $\bar{M}\bar{Y}\bar{\Gamma}\bar{X}$:

$$
\chi_y = \frac{1}{\pi} \sum_{j=1}^{n_{\text{occ}}/2} \left[ \theta_j^+(\bar{M}) - \theta_j^+(\bar{X}) + \int_{\bar{M}\bar{Y}} d\theta_j^+ + \int_{\bar{\Gamma}\bar{X}} d\theta_j^+ \right]
+ \sum_{j=1}^{n_{\text{occ}}} \frac{1}{2\pi} \int_{\bar{Y}\bar{\Gamma}} d\theta_j \mod 4
$$

(7.3.2)

where $n_{\text{occ}}$ is the number of occupied bands, the superscript $\pm$ indicates the glide sector, and the absence of a superscript indicates the line where $g_y$ is not a symmetry and the sum is over all bands. In the presence of an additional glide, $g_x$, one can obtain $\chi_x$ by the transformation $x \leftrightarrow y, \bar{X} \leftrightarrow \bar{Y}$ in Eq. (7.6.33). Though Eq. (7.6.33) is quite complicated, $(\chi_x, \chi_y)$ can be easily evaluated by considering the bands within each glide sector which cross an arbitrary horizontal line in the Wilson spectrum, as detailed in the supplement. Wallpaper group $p4g$ also has $C_{4z}$ symmetry, which requires $\chi_x = \chi_y$ and implies the existence of the symmorphic mirrors, $\{M_{110}\frac{1}{2}\frac{1}{2}\}$ and $\{M_{110}\frac{1}{2}\frac{1}{2}\}$. The mirrors yield $\mathbb{Z}$ mirror Chern numbers, $n_{110}, n_{110}$, respectively, which satisfy $(-1)^{n_{110}} = (-1)^{n_{110}} = (-1)^{\chi_x}$.

To enumerate the allowed topological phases shown in Fig. 7.2, we consider possible restrictions on $(\chi_x, \chi_y)$. Though $\chi_{x/y}$ can individually take on values 0, 1, 2, 3, only pairs that satisfy $\chi_x + \chi_y \mod 2 = 0$ are permitted in bulk insulators; This can be understood as follows: if $\chi_x + \chi_y$ is odd, the 2D surface consisting of the four partial planes $(0 \leq k_x \leq \pi, 0(\pi), k_z)$ and $(0(\pi), 0 \leq k_y \leq \pi, k_z)$ possesses an overall Chern number, which implies the existence of a gapless point [6, 53], contradicting our original assumption that the system is insulating. We present a rigorous proof
in the supplement, and show that the remaining collection of eight insulating phases forms the group $\mathbb{Z}_4 \times \mathbb{Z}_2$.

For $\chi_{x,y} = 1, 3$, the system is a strong topological insulator (STI). These four “double-glide spin Hall” phases possess the usual two-fold degenerate Kramers pairs at $\bar{\Gamma}, \bar{X},$ and $\bar{Y}$ as well as a four-fold degenerate Dirac point at $\bar{M}$. The four STI phases are topologically distinct, but will appear indistinguishable in ARPES experiments. However, if two double-glide spin hall systems with differing $\chi_{x/y}$ are coupled together, the resulting surface modes will distinguish between $\chi_{x/y} = 1, 3$ [185, 252] (see supplement).

When $\chi_{x,y} = 0, 2$, the system is in a topological crystalline phase. For $(\chi_x, \chi_y) = (0, 2)$ or $(2, 0)$, which is only permitted in a $C_{4z}$-broken surface $pgg$, a variant of the hourglass insulating phase is present on the surface. For example, when $(\chi_x, \chi_y) = (0, 2)$, either time-reversed partners of two-fold degenerate free fermions live along $\bar{\Gamma} \bar{X}$ or both two-fold degenerate fermions live along $\bar{\Gamma} \bar{Y}$ and a four-fold degenerate Dirac fermion exists at $\bar{M}$.

Finally, for $\chi_x = \chi_y = 2$, we find that the system exists in a previously un-characterized “topological Dirac insulating” phase, capable of hosting just a single four-fold degenerate Dirac surface fermion at $\bar{M}$.
7.4 Discussion

We have demonstrated the existence of a topological Dirac insulator – a topological crystalline material with a single four-fold degenerate surface Dirac point stabilized by two perpendicular glides. This is one of eight topologically distinct phases that can exist in insulating orthorhombic crystals with surfaces that preserve two perpendicular glides; we have classified the eight phases by the topological indices $(\chi_x, \chi_y)$ that characterize the connectivity of the $z$-projection Wilson loop spectrum. After an exhaustive study of the 17 wallpaper groups, these phases are revealed to be the final theoretically undiscovered 3D time-reversal-symmetric bulk topological insulating phases.

We also find that there exists a simple intuition for the topological crystalline phases $\chi_{x,y} = 0, 2$. In the supplement, we present a simple eight-band tight-binding model which, when half-filled, can be tuned to realize all $\mathbb{Z}_4 \times \mathbb{Z}_2$ double-glide insulating phases. In a particular regime of phase space, where the spin-orbit coupling terms at the $\bar{X}$ and $\bar{Y}$ points are absent and bulk inversion symmetry is imposed, the Wilson loop eigenvalues at the edge TRIMs are pinned to $\pm 1$ ($\theta(\bar{M}/\bar{X}/\bar{Y}) = 0, \pi$) and each TRIM represents the end of a doubly-degenerate SSH model. In this limit, when the product of parity eigenvalues at the $\bar{\Gamma}$ point satisfies $\xi(\bar{\Gamma}) = +1$, the allowed crystalline connectivities are exactly the relative polarizations between the SSH chains, and $\chi_{x,y} = 2\{((1/\pi)[\theta(\bar{M}) - \theta(\bar{Y}, \bar{X})] \mod 2}\}$. Further details of this calculation are provided in the supplement.
Finally, as the $(2,2)$ topological surface Dirac point is symmetry-pinned to the QCP between a 2D TI and a NI, we examine its potential for hosting strain-engineered topological physics. Consider the two-site surface unit cell in wallpaper group $pgg$ from Fig. 7.1. In the $(2,2)$ topological Dirac insulating phase, the surface Dirac fermion can be captured by the $k \cdot p$ Hamiltonian:

$$H_{\vec{M}} = \tau^x (v_x \sigma^x k_x + v_y \sigma^y k_y)$$ (7.4.1)

where $\tau$ is a sublattice degree of freedom, $\sigma$ is a $T$-odd orbital degree of freedom, and $g_{x/y} = \tau^y \sigma^{x/y}$. There exists a single, $T$-even, mass term, $V_m = m \tau^z$, which satisfies $\{H_{\vec{M}}, V_m\} = 0$ and is therefore guaranteed to fully gap $H_{\vec{M}}$. Therefore, surface regions with differing signs of $m$ will be in topologically distinct gapped phases and must be separated by 1D topological QSH surface domain walls, protected only by time-reversal symmetry[98]. As $\vec{M}$ is in point group $2mm$ and $\{V_m, g_{x/y}\} = 0$, $V_m$ can be considered an $xy A_2$ distortion, or one which could be achieved by strain in the $x + y$ direction and compression in the $x - y$ direction[203].

Furthermore, under the right interacting conditions or chemical modifications, a topological Dirac insulator surface can reconstruct and self-induce this mass term. In this case, one could imagine a system with a random distribution of regions of varying $\pm m$, separated by a network of 1D QSH domain walls. These domain wall networks would appear qualitatively similar to those proposed in bilayer graphene[35, 101, 161, 163, 223, 254]. However, whereas those domain walls
are protected by sublattice symmetry and are therefore quite sensitive to disorder, domain walls originating from topological Dirac insulators are protected by only time-reversal symmetry, and therefore should be robust against surface disorder.

7.5 Chapter Acknowledgments

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7.6 Supplemental Material

7.6.1 Fermion Doubling in 2D Crystals

In this section, we discuss how fermion doubling theorems in 2D constrain band structures and how apparent exceptions to them manifest on the surfaces of bulk 3D topological phases. To be precise, we will use the phrase “Dirac fermion” only to refer to four-fold-degenerate linearly dispersing fermions, in either two or three dimensions. In this nomenclature, the surface states of a topological insulator
are therefore not “Dirac points,” but are two-fold-degenerate linearly dispersing fermions by another name (in a topological insulator they are linearly dispersing Kramers pairs). By making this choice of nomenclature, we preserve the designation of the linear fermions in graphene as Dirac points. Furthermore, as we will show in this appendix, Dirac points are crystalline-symmetry-pinned to the quantum critical point between a topological and a trivial insulator.

7.6.1.1 2D Fermion Doubling for Two-fold-degenerate linear fermions

In 2D, a system may host linearly-dispersing two-fold-degenerate fermions. Such gapless fermions may exist as fine-tuned points or, if additional symmetries are present to protect them, may exist in a stable phase. Here, we are interested in stable phases. Thus, we restrict ourselves to only discussing systems for which all possible symmetry-allowed hopping terms have been included. For example, the critical point separating two topologically distinct insulating phases in a two-band model features a two-fold-degenerate gapless fermion. However, without imposing additional symmetries, this fermion can be gapped, and, generically, the system will be insulating at half-filling.

The simplest example of a symmetry protecting a two-fold linear fermion occurs in a crystal with time-reversal symmetry, $\mathcal{T}$, satisfying $\mathcal{T}^2 = -1$. This requires states to be two-fold-degenerate at the Time-Reversal-Invariant-Momenta (TRIMs) by Kramers’s theorem. Two-fold-degenerate fermions can also appear pairwise along
high-symmetry lines and, if the system is a layer group, along planes, with symmetry stabilization coming from a combination of crystalline and time-reversal symmetries.

In 2D systems, these symmetry-protected gapless points come in pairs, a consequence of the parity anomaly\[14, 97, 177\]. We illustrate this result in the case of a single two-fold-degenerate linear fermion protected by time-reversal symmetry, $\mathcal{T} = i\sigma^y K$, described by the following 2D $k \cdot p$ theory:

$$\mathcal{H} = v_x k_x \sigma^x + v_y k_y \sigma^y. \quad (7.6.1)$$

There is a single remaining Pauli matrix, $\sigma^z$, which anticommutes with all of the terms in Eq. (7.6.1) and opens a gap. The mass term $V_m = m \sigma^z$ breaks $\mathcal{T}$ symmetry and gaps locally to a $k \cdot p$ theory of a Chern insulator, with two bands of winding number $C$ and $C + 1$, respectively, for some $C \in \mathbb{Z}$. If (7.6.1) is a complete description of the low-energy physics, a contradiction arises: because $\{V_m, \mathcal{T}\} = 0$, the two gapped phases that result from choosing opposite signs of $m$ are related to each other by transformation under $\mathcal{T}$. In particular, the band with Chern number $C$ when $m > 0$ is related to the band with Chern number $C + 1$ when $m < 0$. Since $C$ is odd under time reversal, $-C = C + 1$. This condition cannot be satisfied by $C \in \mathbb{Z}$.

Thus, the hypothesis that (7.6.1) is a complete description of the low-energy physics cannot be true. For a system with a single two-fold fermion, even at $V_m = 0$, time-reversal symmetry becomes spontaneously (anomalously) broken due to the
existence of the degeneracy point, and the system forms an anomalous Hall state with $|C| = 1/2$. In order for time reversal to remain unbroken, there must be a compensating second degeneracy point somewhere else in the Brillouin zone, also with $|C| = 1/2$. The only details of time-reversal symmetry that entered into the preceding argument are that $\mathcal{T}V_m\mathcal{T}^{-1} = -V_m$, and so the general result remains true for any symmetry that protects a gapless fermion in 2D.\footnote{This is due to the fact that a Pauli-Villars regulator is a function of $V_m$, and so this regularization must break the symmetry, and so we derive the same anomaly-generating functional as in the literature.}

We can gain some further intuition about the parity anomaly by noting that the anomalous hall conductance $C$ is related to the Berry phase at the Fermi surface by\cite{81}

$$C = \frac{1}{2\pi i} \log \exp i \oint_{FS} \mathbf{A} \cdot d\mathbf{k}$$ \hspace{1cm} (7.6.2)

Let us take a compact Brillouin zone with $N$ gapless fermions, and let the Fermi level be above all bands. By evaluating the Berry phase we find that $2\pi i C = \log((-1)^N)$. However, in this setup we also have that $C$ is the total Chern number of all bands, and hence $C \in \mathbb{Z}$. Thus we conclude $N \in 2\mathbb{Z}$. In the context of three-dimensional topological insulators, we note that each surface taken in isolation is a 2D system with a single gapless fermion. From the above discussion we thus recover the well-known result that each surface of a topological insulator has a half-quantized anomalous Hall conductivity, and that only when both surfaces are connected by a bulk can the system be described in an anomaly-free way\cite{61, 153, 170}.
The same logic can be applied to a 3D material by replacing the mass term \( m\sigma^z \) by \( k_z \sigma^z \); in this case the gapless point would be a Weyl point of Chern number +1 and the two gapped Hamiltonians of opposite-signed mass lie in the planes above and below it. This expresses the so-called “descent relation” between the parity anomaly in two dimensions and the chiral anomaly in three dimensions.[15] The doubling theorem then requires that the low-energy physics cannot be described by only a single Weyl point: there must be another Weyl point or other band crossing at the Fermi level. In 3D, this is the celebrated Nielsen-Ninomiya theorem[158].

7.6.1.2 2D Fermion Doubling for Dirac fermions

We now extend these arguments to show why four-fold-degenerate 2D Dirac fermions cannot be stabilized as the only nodal features at a given energy. As in the two-fold degenerate case, while many models might display Dirac fermions upon fine-tuning, here we are interested in robust Dirac fermion phases. Thus, we only consider systems that display Dirac fermions when all symmetry-allowed hopping terms are present. The crux of the arguments in this section was originally highlighted in Refs. 65, 245.

When Dirac points occur off of the TRIMs, time-reversal requires that they come in pairs. For these \( \mathcal{T} \)-paired Dirac fermions the preceding discussion can easily be generalized, and follows by relating the gapping of the 2D Dirac point to the \( \mathbb{Z}_2 \) index, in much the same way as we did above for Chern numbers and Weyls [239].

280
Just as the Chern number jumps by one as a plane in 3D passes a Weyl point, the $\mathbb{Z}_2$ index flips when a plane passes a Dirac fermion at a low-symmetry $k$-point.

In other cases, the Dirac points which occur in 2D are filling-enforced and pinned to the TRIMs by crystalline symmetries and time-reversal. As shown in Ref. 221, these filling-enforced, high-symmetry Dirac points can only occur in 2D systems where either inversion anticommutes with a two-fold non-symmorphic symmetry or where two perpendicular non-symmorphic symmetries anticommute, such as the two glides in $pgg$.

Consider first a 2D spinful system with inversion symmetry, denoted $\mathcal{I}$, and a screw, $s_{2y} = t_{x/2}C_{2y}$. At $k_x = \pi$, $\mathcal{I}^2 = s_{2y}^2 = +1$ and $\{\mathcal{I}, s_{2y}\} = 0$. In a time-reversal-invariant system, these symmetries require a four-dimensional representation: more generally, for any Hamiltonian invariant under two symmetries, $A$ and $B$, in addition to $\mathcal{T}$, such that $\{A, B\} = [A, \mathcal{T}] = [B, \mathcal{T}] = 0$ and $A^2 = 1$, any eigenstate of the Hamiltonian, $\psi$, which is also an eigenstate of $A$, is part of a four-fold degenerate quartet of orthogonal states, $\psi, \mathcal{T}\psi, B\psi, \mathcal{T}B\psi$. In our example, there is a four-fold degeneracy at each TRIM with $k_x = \pi$. In general, the combination of $\mathcal{I}$ and a two-fold non-symmorphic symmetry will always mandate that there are no fewer than two Dirac points for a given filling: since $\mathcal{I}$ anti-commutes with the non-symmorphic symmetry at two of the TRIMs in 2d and $\mathcal{I}^2 = +1$, there are always at least two TRIM points with four-fold degeneracies.

In the case where there are two perpendicular nonsymmorphic symmetries, but
no inversion symmetry, the obstruction to forming an isolated, stable Dirac fermion takes a slightly different form. Consider the trivial phase of wallpaper group \( pgg \), for example, which is characterized by \( T \) and two glides, \( g_{x,y} = \{ M_{x,y} | \frac{1}{2}, \frac{1}{2} \} \). At \( k_x = k_y = \pi \), \( \{ g_x, g_y \} = 0 \) and \( g_x^2 = g_y^2 = +1 \), and therefore a Dirac point exists. However, this condition is only met at this corner TRIM, and no other four-fold degeneracies are allowed elsewhere in this system. In this case, the Dirac point is obstructed from being alone by the filling-enforced hourglass structures also required to exist by the presence of singly-degenerate eigenstates of \( g_{x,y} \). In these systems, the Dirac point occurs at the same filling as four 2D Weyl points, and is also prevented from being alone and stable at any filling.

We pose an explanation for this obstruction in similar terms to the resolution of the parity anomaly of the previous section. Suppose a combination of symmetries were to allow a single stable Dirac point. The \( k \cdot p \) model Hamiltonian at a corner TRIM in our previous system with \( I \) and \( s_{2y} \) is described by a linear \( k \cdot p \) model:

\[
\mathcal{H} = v_x k_x \tau^x \sigma^y + k_y [v_{y1} \tau^y + v_{y2} \tau^x \sigma^x + v_{y3} \tau^x \sigma^z]
\]  

(7.6.3)

where \( I = \tau^z \), \( s_{2y} = \tau^y \sigma^y \), and \( T = i \sigma^y K \). The four Dirac matrices present in \( \mathcal{H} \) span the space of symmetry-allowed matrices. Thus, the system supports a robust four-fold-degenerate gapless fermion stabilized by crystal-symmetries.

As before, we can examine the consequences of locally breaking one of the symmetries. To guarantee that the \( k \cdot p \) Hamiltonian is gapped everywhere, we seek
a mass term to anticommute with all of the terms in $\mathcal{H}$. Generically, the Clifford algebra of Dirac matrices is spanned by four $\mathcal{T}$-odd matrices which couple to crystal momenta, and one $\mathcal{T}$-even matrix, here $V_m = m\tau^z$. For either sign of $m$, the resulting phase is 2D and $\mathcal{T}$-symmetric. This takes the form of a Jackiw-Rebbi problem: the existence of a single $\mathcal{T}$-allowed mass term requires that the gapped phases characterized by different signs of $m$ have different topological indexes. As the only available index for this dimensionality in the presence of strong spin-orbit-interaction is the $\mathbb{Z}_2$ QSH invariant, then this requires that at the $\mathbf{k} \cdot \mathbf{p}$ level, the two gapped Hamiltonians have different QSH indexes $n = 0, 1$.

To show the need for fermion doubling, we expand to the full BZ of a hypothetical system where this fermion is the only feature at the Fermi energy and show that there is a contradiction. We label the Bloch wavefunctions of the phase when $m > 0$ by $|u(k)\rangle$ and those of the phase with $m < 0$ by $|\tilde{u}(\tilde{k})\rangle = s_{2y}|u(k)\rangle$, where $\tilde{k} = s_{2y}k$. The integral of the pfaffian of the matrix $w_{ij} = \langle u(-k)_{i}|\mathcal{T}|u(k)_{j}\rangle$ gives the QSH $\mathbb{Z}_2$ topological invariant [107]. Consider relating this matrix for one gapped phase to the other by the operation of the broken symmetry, $s_{2y}$: $\tilde{w}_{ij} = \langle u(-k)_{i}|\mathcal{T}s_{2y}^\dagger s_{2y}|u(k)_{j}\rangle = \langle u(-k)_{i}|\mathcal{T}s_{2y}^\dagger s_{2y}|u(k)_{j}\rangle = w_{ij}$ because $[\mathcal{T}, s_{2y}] = 0$. Therefore, having the same $w$ matrix, the two phases have the same QSH invariant, contradicting the earlier Jackiw-Rebbi requirement that the two insulating phases are topologically distinct.

The resolution of this is a fermion doubling requirement for 2D four-fold-degenerate Dirac points. Specifically, a closed 2D crystal cannot host a single symmetry-
stabilized Dirac point at the Fermi level. In the cases where the Fermi surface is gapped except for exactly two Dirac points, each Dirac point can have a single \( T \)-symmetric mass term \( m_{1,2} \) such that the overall \( Z_2 \) QSH invariant, \( n \), satisfies 

\[
\begin{align*}
  n &= \frac{1}{2} [\text{sgn}(m_1) - \text{sgn}(m_2)] \mod 2.
\end{align*}
\]

Under transforming by the broken symmetry operation, the signs of both \( m_{1,2} \) are flipped and \( n \) is preserved [245].

Like the topological insulator before it, the topological Dirac insulator that we present in this chapter “cheats” this fermion doubling by placing each of its two Dirac points on opposite surfaces of a 3D bulk. While they each live alone on a surface, and therefore pin that surface to a 2D QSH transition, the Dirac points (or a Dirac point and four Weyl points) in the combined system of two opposing surfaces respect the fermion doubling requirement.

### 7.6.2 Symmetries and Degeneracies of Wallpaper Groups \( pgg \) and \( p4g \)

The wallpaper, or plane, groups describe the 17 possible configurations of symmetries on the two-dimensional surface of a three-dimensional, time-reversal-symmetric crystal [44]. Of these groups, only two have multiple nonsymmorphic symmetries.[26] Specifically, wallpaper groups \( pgg \) and \( p4g \) contain glide lines in the \( x \) and \( y \) (surface in-plane) directions; \( p4g \) has an additional \( C_4 \) symmetry that is not present in \( pgg \).

The group \( pgg \) is generated entirely by the two glides:

\[
g_{x,y} = \{ M_{x,y} | \begin{array}{c} 1 \\ 1 \\ 2 \end{array} \},
\]

(7.6.4)
Figure 7.3: The 2D surface Brillouin zone for wallpaper group $pgg$. Bands with glide eigenvalue $\lambda^+ (\lambda^-)$ are drawn as solid (dashed) lines. Bands along lines of type (a) are singly degenerate eigenstates of $g_{x/y}$ and therefore are restricted to either form hourglass or Quantum Spin Hall connectivities along $\bar{\Gamma} \bar{X}$ and $\bar{\Gamma} \bar{Y}$. Along lines of type (b), bands are two-fold degenerate because they are invariant under the combined operation $(g_{y/x} T)^2 = -1$; since such pairs have opposite $g_{x/y}$ eigenvalues, generically lines cannot cross to form four-fold degeneracies at low-symmetry points along this line. However, at (c), the $M$ point, bands meet and form a fourfold-degenerate 2D Dirac point. Bands in wallpaper group $p4g$ behave the same way, with the additional restriction from $C_{4z}$ symmetry that bands along $\bar{\Gamma} \bar{X}$ and $\bar{\Gamma} \bar{Y}$ form the same connectivities.

while wallpaper group $p4g$ is generated by

$$g_x = \{M_x \frac{1}{2}, \frac{1}{2}\}, \quad C_{4z} = \{C_{4z} | 00\}.$$  \hspace{1cm} (7.6.5)

The product of the two generators for $p4g$ yields two additional symmorphic mirror symmetries, $\{m_{x+y} | \frac{1}{2}, \frac{1}{2}\}$ and $\{m_{x-y} | \frac{1}{2}, \frac{1}{2}\}$. Though containing translations, these symmetries are still symmorphic as $\{m_{x \pm y} | \frac{1}{2}, \pm \frac{1}{2}\}$ leaves the line $y = \pm (-x + \frac{1}{2})$ invariant. In Figure 7.1, we show the locations of the glides, mirrors, and $C_{4z}$ rotation centers for both wallpaper groups realized with a two-site unit cell.

In crystal momentum space the symmetry generators enforce required band groupings along lines and at points. In Figure 7.3, we show one quarter of the
surface BZ and identify relevant lines and points with the letters (a), (b), and (c). Lines sharing the same letter obey the same symmetry restrictions, though for wallpaper group \( pgg \), which lacks a \( C_{4z} \) symmetry, they may individually display different features.

The lines designated (a) in Fig. 7.3 are \( \bar{\Gamma} \bar{X} \) and \( \bar{\Gamma} \bar{Y} \) and host singly degenerate bands which are eigenstates of \( g_y \) or \( g_x \), respectively. As detailed extensively in Refs. 9, 214, 221, 245, singly-degenerate bands along lines invariant under a glide form hourglass or Quantum Spin Hall flows.

Bands along lines designated (b), \( \bar{X} \bar{M} \) and \( \bar{Y} \bar{M} \), are also eigenstates of \( g_x \) or \( g_y \), respectively. However, unlike the lines in (a), they are doubly degenerate, because the symmetry operation \( T g_y (T g_x) \) leaves the line \( \bar{X} \bar{M} (\bar{Y} \bar{M}) \) invariant and squares to \(-1\). We now show that all potential band crossings along the line \( \bar{X} \bar{M} \) are avoided by utilizing the fact that bands along this line are also eigenstates of \( g_x \). If \( g_x |+\rangle = i e^{i k_y/2} |+\rangle \), then, using the commutation relation \( g_x g_y = -g_y g_x t_x t_y \),

\[
g_x (T g_y |+\rangle) = -T g_y g_x t_x t_y |+\rangle = T g_y i e^{-i k_y/2} |+\rangle = -i e^{i k_y/2} (T g_y |+\rangle)
\] (7.6.6)

Thus, the Kramers partners \( |+\rangle \) and \( g_y T |+\rangle \) have opposite \( g_x \) eigenvalues, and we note that eigenstates of \( g_y \) along \( \bar{Y} \bar{M} \) must behave in the same manner by \( x \leftrightarrow y \) exchange symmetry. Since all sets of Kramers pairs along line (b) have the same pair of eigenvalues, they belong to the same irreducible representation and so crossings between these bands will generically be avoided.
Finally, at the point $\bar{M}$, labelled (c), bands are four-fold degenerate, a unique property of wallpaper groups $pgg$ and $p4g$. This can be easily seen because the $\bar{M}$ point is invariant under $g_x, g_y$ and $T$. Thus, if $\psi$ is an eigenstate of $g_x$, $\psi, T\psi, g_y\psi$ and $Tg_y\psi$ form a degenerate quartet of states; clearly the Kramers pairs are orthogonal and since the first two states have the opposite $g_x$ eigenvalue as the last two states, they are also orthogonal. This algebra can only be satisfied in the strong spin-orbit coupled wallpaper groups by two perpendicular glides. Therefore a four-fold point degeneracy can only be hosted on the surfaces of three-dimensional objects which satisfy the symmetries of $pgg$ or $p4g$.

We now determine the low-energy band dispersion near a four-fold crossing at (c). Returning to the two-site unit cell depicted in Figure 7.1, we construct a $k \cdot p$ theory around $\bar{M}$. Letting $\tau$ represent the sublattice degree of freedom and $\sigma$ the local spin degree of freedom, we choose the representation $g_{x/y} = \tau^y \sigma^{x/y}$ and $T = i\sigma^y K$. Then, to linear order in $k_{x,y}$, an allowed Hamiltonian is given by,

$$\mathcal{H}_{\bar{M}} = \tau^x (v_x \sigma^x k_x + v_y \sigma^y k_y).$$  \hspace{1cm} (7.6.7)

This is the equation of a linearly-dispersing four-fold-degenerate 2D fermion. Therefore bands at $\bar{M}$ generically form in Dirac points.
7.6.3 Tight-binding notation

Here we provide the tight-binding notation that will be used in subsequent sections, following Ref 9. In the unit cell labelled by the Bravais lattice vector, $\mathbf{R}$, the wavefunction corresponding to an orbital labelled by $\alpha$ at position $\mathbf{R} + \mathbf{r}_\alpha$ is denoted by $|\phi_{\mathbf{R},\alpha}\rangle$. The Fourier transformed operators are given by,

$$
\phi_{\mathbf{k},\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot (\mathbf{R} + \mathbf{r}_\alpha)} |\phi_{\mathbf{R},\alpha}\rangle
$$

(7.6.8)

The single-particular Hamiltonian, $\hat{H}$, defines a tight-binding Hamiltonian,

$$
H(\mathbf{k})_{\alpha,\beta} = \langle \phi_{\mathbf{k},\alpha} | \hat{H} | \phi_{\mathbf{k},\beta} \rangle
$$

(7.6.9)

whose eigenstates are denoted $|u^n(\mathbf{k})\rangle$.

The Fourier transform in Eq (7.6.8) shows that the Hamiltonian is not necessarily invariant under a shift of a reciprocal lattice vector, $\mathbf{G}$. Instead,

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

(7.6.10)

where $\hat{V}(\mathbf{G})_{\alpha\beta} = \delta_{\alpha\beta} e^{i\mathbf{G} \cdot \mathbf{r}_\alpha}$. Thus, we can choose the basis of eigenstates so that

$$
|u^n(\mathbf{k} + \mathbf{G})\rangle = \hat{V}(\mathbf{G})^{-1} |u^n(\mathbf{k})\rangle
$$

(7.6.11)
7.6.3.1 Symmetries

If the lattice is invariant under a spatial symmetry, \( \hat{g} \), that acts in real space by taking \( r \rightarrow D_g r + \delta \), where \( D_g \) is the matrix that enforces a point group operation and \( \delta \) is a (perhaps fractional) lattice translation, then \( \hat{g} \) acts on states by:

\[
\hat{g} |\phi_{\mathbf{R},\alpha}\rangle = |\phi_{\mathbf{R}',\beta}\rangle [U_g]_{\alpha\beta},
\]

(7.6.12)

where \( \mathbf{R}' = D_g(\mathbf{R} + r_\alpha) + \delta - r_\beta \) is a Bravais lattice vector and \( U_g \) is a unitary matrix. It is convenient to define the Fourier transformed operator, \( \hat{g}_k \), which can have explicit \( k \) dependence when it acts on Bloch states, by:

\[
\hat{g}_k |\phi_{\mathbf{k},\alpha}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot (\mathbf{R} + r_\alpha)} \hat{g} |\phi_{\mathbf{R},\alpha}\rangle \\
= \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot (\mathbf{R} + r_\alpha)} |\phi_{D_g(\mathbf{R} + r_\alpha) + \delta - r_\beta,\beta}\rangle [U_g]_{\alpha\beta} \\
= \frac{1}{\sqrt{N}} e^{-i(D_g k) \cdot \delta} \sum_{\mathbf{R}} e^{i(D_g k) \cdot (D_g(\mathbf{R} + r_\alpha) + \delta)} |\phi_{D_g(\mathbf{R} + r_\alpha) + \delta - r_\beta,\beta}\rangle [U_g]_{\beta\alpha} \\
= e^{-i(D_g k) \cdot \delta} |\phi_{D_g k,\beta}\rangle [U_g]_{\alpha\beta},
\]

(7.6.13)

Thus, \( \hat{g}_k \) separates into a product of a \( k \)-dependent phase and a matrix, \( U_g \), that rotates the orbitals:

\[
\hat{g}_k = e^{-i(D_g k) \cdot \delta} U_g
\]

(7.6.14)
If $\hat{H}$ is invariant under $\hat{g}$, then Eq (7.6.13) shows:

$$H(k) = g_k^\dagger H(D_g k) g_k$$  \hspace{1cm} (7.6.15)

We can follow the same procedure for an anti-unitary operator, $\mathcal{T}_g \equiv \mathcal{T}\hat{g}$, to find

$$\mathcal{T}_{g,k} \equiv e^{i(D_g k)\delta} U_{T_g K},$$  \hspace{1cm} (7.6.16)

where $K$ is the complex conjugation operator. Similarly to Eq (7.6.15),

$$H(k) = \mathcal{T}_{g,k}^{-1} H(-D_g k) \mathcal{T}_{g,k}$$  \hspace{1cm} (7.6.17)

### 7.6.3.2 Projector onto occupied states

We define the projector onto the $n_{\text{occ}}$ occupied states,

$$\hat{P}(k) = \sum_{n=1}^{n_{\text{occ}}} |u^n(k)\rangle \langle u^n(k)|,$$  \hspace{1cm} (7.6.18)

which satisfies, using Eq (7.6.11),

$$\hat{P}(k) = \hat{V}(G) \hat{P}(k + G) \hat{V}(G)\dagger.$$  \hspace{1cm} (7.6.19)

Given a spatial symmetry, $\hat{g}$, Eq (7.6.15) shows that $\hat{g}_k |u^n(k)\rangle$ has the same energy as $|u^n(k)\rangle$. Hence, the projector onto the occupied states at momentum
$D_g k$ is given by,

$$ \hat{P}(D_g k) = \sum_{n=1}^{n_{\text{occ}}} \hat{g}_k |u^n(k)\rangle\langle u^n(k)| \hat{g}_k^\dagger = \hat{g}_k \hat{P}(k) \hat{g}_k^\dagger \quad (7.6.20) $$

In subsequent sections, we will want to know how $\hat{g}_{k+G}$ is related to $\hat{g}_k$. Plugging Eq (7.6.10) into Eq (7.6.15):

$$ \hat{g}_k \hat{V}(G) \hat{H}(k+G) \hat{V}(G)^\dagger \hat{g}_k^{-1} = \hat{V}(D_g G) \hat{H}(D_g(k+G)) \hat{V}(D_g G)^\dagger \quad (7.6.21) $$

Thus,

$$ \hat{g}_{k+G} = \hat{V}(D_g G)^\dagger \hat{g}_k \hat{V}(G) \quad (7.6.22) $$

For an anti-unitary symmetry, $\mathcal{T}_g \equiv \mathcal{T} \hat{g}$, the analogous equations are:

$$ \hat{P}(-D_g k) = \sum_{n=1}^{n_{\text{occ}}} |\mathcal{T}_{g,k} u^n(k)\rangle\langle \mathcal{T}_{g,k} u^n(k)| \quad (7.6.23) $$

and

$$ \mathcal{T}_{g,k+G} = \hat{V}(-D_g G)^\dagger \mathcal{T}_{g,k} \hat{V}(G) \quad (7.6.24) $$

### 7.6.4 Wilson loops

A precise way to distinguish the distinct surface connectivities is obtained through the eigenvalues of Wilson loops, which, as we will elaborate, also gives information
about the edge state spectrum.\[7, 9, 64, 180, 187, 194, 246\] Here, we are interested in the Wilson loop matrix,

\[ W_{(k_x, k_y, k_z_0)} \equiv V(2\pi \hat{z}) P e^{i \int_{k_z_0}^{k_z_0+2\pi} dk_z A_z(k_z, k_y, k_z)}, \tag{7.6.25} \]

where \( P \) indicates that the integral is path-ordered, \( A_z(k)_{ij} \equiv i \langle u^i(k) | \partial_{k_z} u^j(k) \rangle \) is a matrix whose rows and columns correspond to filled bands, and \( V \) is the gauge transformation defined in Eq (7.6.11), where \( 2\pi \hat{z} = (0, 0, 2\pi) \). The eigenvalues of \( W \) are gauge invariant and of the form \( e^{i\theta(k_x, k_y)} \), i.e., they are independent of the ‘base point,’ \( k_z_0 \).

In this appendix, we show that a space group with two glides, \( g_{x,y} \equiv \{ M_{x,y} | 1 \frac{1}{2} 0 \} \), as well as time reversal symmetry, \( T \), has the following constraints on its Wilson loop eigenvalues:

- Along the lines \((k_x, \pi)\) and \((\pi, k_y)\), the Wilson loop eigenvalues are doubly-degenerate, due to the anti-unitary symmetries \( g_x T \) and \( g_y T \), respectively (see Sec 7.6.4.2).

- At the \((\pi, \pi)\) point, the doubly-degenerate bands meet at a four-fold band crossing (see Sec 7.6.4.3).

- Along the \( \bar{X} \bar{M}(\bar{Y} \bar{M}) \) and \( \bar{\Gamma} \bar{Y}(\bar{\Gamma} \bar{X}) \) lines, bands can be labeled by the \( g_x(g_y) \) eigenvalue (see Sec 7.6.4.3).
The band structures shown in the main text are also plots of the phase, \( \theta(k_x, k_y) \), of the Wilson loop eigenvalues; the vertical axis is the \( \theta \) axis and runs from 0 to \( 2\pi \). The gauge invariance of the loops allows us to write down a topological invariant that distinguishes the states, as derived in Appendix 7.6.5.1.

### 7.6.4.1 Discretized Wilson loop

For completeness, following Ref 9, we derive a discretized version of the Wilson loop (7.6.25), which is useful for clarity when deriving symmetry constraints. Using the projector onto occupied states, \( \hat{P} \), defined in Eq (7.6.18), we derive the discretized Wilson loop matrix,

\[
[W_{(k_\perp,k_0)}]_{nm} \equiv \left[ V(2\pi \hat{z}) P e^{i\frac{k_{z0}}{N} + 2\pi dk_z A_z(k_\perp,k_z)} \right]_{nm}
\]

\[
\approx \left[ V(2\pi \hat{z}) P e^{i\frac{2\pi}{N} \sum_{j=1}^{N} A_z(k_\perp,k_{z0} + \frac{2\pi j}{N})} \right]_{nm}
\]

\[
\approx \left[ V(2\pi \hat{z}) P \prod_{j=1}^{N} \left( 1 + \frac{2\pi j}{N} A_z(k_\perp,k_{z0} + \frac{2\pi j}{N}) \right) \right]_{nm}
\]

\[
\approx V(2\pi \hat{z})_{nnN} P \prod_{j=1}^{N} \left( \delta_{n,n_j-1} - \frac{2\pi}{N} \langle u^n_j(k_\perp,k_{z0} + \frac{2\pi j}{N}) | \partial_{k_z} u^{n_j-1}(k_\perp,k_{z0} + \frac{2\pi j}{N}) \rangle \right)
\]

\[
\approx V(2\pi \hat{z})_{nnN} P \prod_{j=1}^{N} \langle u^n_j(k_\perp,k_{z0} + \frac{2\pi j}{N}) | u^{n_j-1}(k_\perp,k_{z0} + \frac{2\pi (j-1)}{N}) \rangle
\]

\[
\approx \langle u^n(k_\perp,k_{z0}) | V(2\pi \hat{z}) \hat{\Pi}(k_\perp,k_{z0}) | u^m(k_\perp,k_{z0}) \rangle \quad (7.6.26)
\]

where \( k_\perp \equiv (k_x, k_y) \). The approximations become exact in the \( N \to \infty \) limit. In the intermediate lines, the \( n_j \) are implicitly summed over filled bands and \( n_0 = m \);
in the last line we have defined the ordered product of projectors,

\[ \hat{\Pi}(k_\perp, k_z) \equiv \hat{P}(k_\perp, k_z + 2\pi) \hat{P}(k_\perp, k_z + \frac{2\pi(N-1)}{N}) \cdots \hat{P}(k_\perp, k_z + \frac{2\pi}{N}) \quad (7.6.27) \]

Eq (7.6.26) shows that the discretized Wilson loop can be written in the basis-invariant form,

\[ \mathcal{W}_{(k_\perp, k_z)} = \hat{V}(2\pi \hat{z}) \hat{\Pi}(k_\perp, k_z) \quad (7.6.28) \]

By applying Eq (7.6.19) to (7.6.28), for a reciprocal lattice vector \( G = (G_\perp, 0) \),

\[ \mathcal{W}_{(k_\perp + G_\perp, k_z)} = \hat{V}(G_\perp, 0)^\dagger \mathcal{W}_{(k_\perp, k_z)} \hat{V}(G_\perp, 0), \quad (7.6.29) \]

i.e., the Wilson loop eigenvalues are invariant under shifts of \((G_\perp, 0)\).

### 7.6.4.2 Effect of time-reversal-like symmetries on the Wilson loop

Here, we consider an anti-unitary symmetry, \( T_g \equiv \hat{T}_g \), which satisfies \( T_g^2 = -1 \), flips the sign of \( k_z \) and does not translate in the \( \hat{z} \) direction, i.e., \( -D_g(k_\perp, k_z) = (-D_gk_\perp, -k_z) \), and \( \delta = (\delta_x, \delta_y, 0) \). Using Eq (7.6.16), these properties imply \( T_g^2 = -1 \) and \( T_g(k_\perp, k_z) = T_g(k_\perp, 0) \equiv T_gk_\perp \). We would like to relate \( \mathcal{W}_{(-D_gk_\perp, 0)} \) to \( \mathcal{W}_{(k_\perp, 0)} \),
to which end we compute:

\[
\langle u^m(k_\perp,0) | (T_{g,k_\perp} \mathcal{W}_{(-D_gk_\perp,0)} T_{g,k_\perp})^\dagger | u^n(k_\perp,0) \rangle \\
= -\langle T_{g,k_\perp} u^n(k_\perp,0) | \mathcal{W}_{(-D_gk_\perp,0)} T_{g,k_\perp} u^m(k_\perp,0) \rangle \\
= -\langle T_{g,k_\perp} u^n(k_\perp,0) | \hat{V}(2\pi \mathbf{\hat{z}}) \hat{\Pi}(-D_gk_\perp,0) T_{g,k_\perp} u^m(k_\perp,0) \rangle \\
= -\langle T_{g,k_\perp} u^n(k_\perp,0) | \hat{V}(2\pi \mathbf{\hat{z}}) \hat{P}(-D_gk_\perp,2\pi) \hat{\Pi}(k_\perp,2\pi - \frac{2\pi}{N}) \hat{\Pi}(k_\perp,2\pi - 2\pi) \\
\cdots \hat{\Pi}(k_\perp,2\pi - 2\pi) | u^m(k_\perp,0) \rangle \\
= -\left( \langle u^n(k_\perp,0) | \hat{V}^\dagger(2\pi \mathbf{\hat{z}}) \hat{\Pi}(k_\perp,2\pi - 2\pi) \hat{\Pi}(k_\perp,2\pi - 2\pi) \\
\cdots \hat{\Pi}(k_\perp,2\pi - 2\pi) | u^m(k_\perp,0) \rangle \right)^* \\
= -\left( \langle u^n(k_\perp,0) | \hat{\Pi}(k_\perp,2\pi - 2\pi) \hat{\Pi}(k_\perp,2\pi - 2\pi) \\
\cdots \hat{\Pi}(k_\perp,2\pi - 2\pi) | u^m(k_\perp,0) \rangle \right)^* \\
= -\langle u^m(k_\perp,0) | \hat{V}(2\pi \mathbf{\hat{z}}) \hat{\Pi}(k_\perp,0) | u^n(k_\perp,0) \rangle = -\langle u^m(k_\perp,0) | \mathcal{W}_{(k_\perp,0)} | u^n(k_\perp,0) \rangle
\]

(7.6.30)

We conclude, \(-T_{g,k_\perp} \mathcal{W}_{(-D_gk_\perp,0)} T_{g,k_\perp} = \mathcal{W}_{(k_\perp,0)}^\dagger\). Thus, if \(\psi(k_\perp)\) is an eigenvector of \(\mathcal{W}_{(k_\perp,0)}\) with eigenvalue \(e^{i\theta(k_\perp)}\), then \(T_{g,k_\perp} \psi(k_\perp)\) is an eigenvector of \(\mathcal{W}_{(-D_gk_\perp,0)}\) with the same eigenvalue. Furthermore, if for some \(k_\perp\), \(T_g\) leaves \(k_\perp\) invariant up to a reciprocal lattice vector (i.e., \(-D_g(k_\perp,k_z) = (k_\perp + G_\perp, -k_z)\), where \((G_\perp,0)\) is a reciprocal lattice vector), then from Eq (7.6.29), \(\hat{V}(G_\perp)T_{g,k_\perp} \psi(k_\perp)\) is an eigenstate of \(\mathcal{W}_{(k_\perp,0)}\), also with the same eigenvalue as \(\psi(k_\perp)\). Since \(\hat{V}(G_\perp)T_{g,k_\perp}\) is an antiunitary
symmetry that squares to $-1$, $\psi(k_\perp)$ and $\hat{V}(G_\perp)\mathcal{T}_{g,k_\perp}\psi(k_\perp)$ are orthogonal. Thus, at momenta whose projections onto $(k_x,k_y)$ are invariant under $\mathcal{T}_g$ up to a reciprocal lattice vector, eigenstates of $\mathcal{W}_{(k_z,k_y,0)}$ come in Kramers pairs.

### 7.6.4.3 Effect of unitary symmetries that leave $k_z$ invariant

Here we consider a unitary symmetry, $\hat{g}$, which leaves $k_z$ invariant and does not translate in the $\hat{z}$ direction, i.e., $D_g(k_\perp,k_z) = (D_g k_\perp, k_z)$ and $\delta = (\delta_x,\delta_y,0)$. Using Eq (7.6.13), $g_{(k_\perp,k_z)} = g_{(k_\perp,0)} \equiv g_{k_\perp}$. Eq (7.6.20) shows that $\hat{V}(2\pi \hat{z})\hat{\Pi}(D_g k_\perp, k_z) = \hat{V}(2\pi \hat{z})\hat{g}_{k_\perp} \hat{\Pi}(k_\perp,k_z)\hat{g}_{k_\perp}^\dagger$. Thus, by definition,

$$\mathcal{W}_{(D_g k_\perp,k_z)} = \hat{g}_{k_\perp} \mathcal{W}_{(k_\perp,k_z)} \hat{g}_{k_\perp}^\dagger \quad (7.6.31)$$

Now specialize to momenta invariant under $\hat{g}$ up to a reciprocal lattice vector, so that $D_g(k_\perp,k_z) = (D_g k_\perp,k_z) = (k_\perp + G_\perp,k_z)$, where $(G_\perp,0)$ is a reciprocal lattice vector. At these momenta, $\mathcal{W}_{(D_g k_\perp,k_z)} = \mathcal{W}_{(k_\perp+G_\perp,k_z)}$, which, combined with Eqs (7.6.31) and (7.6.29), shows that at these momenta, $\left[\mathcal{W}_{(k_\perp,k_z)}, \hat{V}(G_\perp)\hat{g}_{k_\perp}\right] = 0$. Thus, at values of $k_\perp$ that are invariant under $D_g$ up to a reciprocal lattice vector, the Wilson loop, $\mathcal{W}_{(k_\perp,k_z)}$, and the operator $\hat{V}(G_\perp)\hat{g}_{k_\perp}$ can be simultaneously diagonalized. Wilson loop bands can be labeled by their $\hat{V}(G_\perp)\hat{g}$ eigenvalue in exactly the same way as energy bands can be labeled by their $\hat{g}_{k_\perp}$ eigenvalue. Thus, we use these terms interchangeably.

296
We now apply the results of this section and the previous section to the glide symmetries defined in the main text, \(g_{x,y} \equiv \{M_{x,y}\}^{-1}\frac{1}{2}\). At \(k_\perp = (\pi, \pi)\), \(D_{g_x}(k_\perp, k_z) = (k_\perp, -2\pi \hat{x})\) and \(D_{g_y}(k_\perp, k_z) = (k_\perp, -2\pi \hat{y})\). From the previous paragraph, the Wilson loop operator \(W_{(k_\perp, k_z)}\) commutes with both \(\hat{V}(-2\pi \hat{x})g_{x,k_\perp}\) and \(\hat{V}(-2\pi \hat{y})g_{y,k_\perp}\), while \(\{\hat{V}(-2\pi \hat{x})g_{x,k_\perp}, \hat{V}(-2\pi \hat{y})g_{y,k_\perp}\} = 0\). Furthermore, from Sec 7.6.4.2, eigenstates of \(W_{(k_\perp, 0)}\) come in Kramers pairs due to time reversal symmetry, which takes \((k_\perp, 0)\) to \((k_\perp, 0) - 2\pi(\hat{x} + \hat{y})\). Thus, if \(\psi(k_\perp)\) is a simultaneous eigenvector of \(W_{(k_\perp, 0)}\) and \(\hat{V}(-2\pi \hat{x})g_{x,k_\perp}\), it forms a quartet with three other states, \(\hat{V}(-2\pi(\hat{x} + \hat{y}))T_{k_\perp} \psi(k_\perp)\), \(\hat{V}(-2\pi \hat{y})g_{y,k_\perp} \psi(k_\perp)\), and \(\hat{V}(-2\pi(\hat{x} + \hat{y}))T_{k_\perp} \hat{V}(-2\pi \hat{y})g_{y,k_\perp} \psi(k_\perp)\), which share the same eigenvalue of \(W_{(k_\perp, 0)}\) but are orthonormal (the orthonormality is verified because the last two states have the opposite \(\hat{V}(-2\pi \hat{x})g_{x,k_\perp}\) eigenvalue as the first two). Thus, the Wilson loop eigenvalues are four-fold degenerate at \(k_\perp = (\pi, \pi)\).

7.6.4.4 Effect of unitary symmetries that flips the sign of \(k_z\)

Here we consider a unitary symmetry, \(\hat{g}\), which flips the sign of \(k_z\) and does not translate in the \(\hat{z}\) direction, i.e. \(D_g(k_\perp, k_z) = (D_g k_\perp, -k_z)\) and \(\delta = (\delta_x, \delta_y, 0)\).

As in the previous section, Eq (7.6.13) guarantees \(g_{(k_\perp, k_z)} = g_{(k_\perp, 0)} \equiv g_{k_\perp}\). Using
Thus, the Wilson loop eigenvalues at $k_\perp$ and $D_g k_\perp$ come in complex conjugate pairs. Consequently, at momenta whose surface projection is invariant (or invariant up to a shift of a reciprocal lattice vector $(G_\perp, 0)$, according to Eq (7.6.29)), the spectrum of the phase of the Wilson loop eigenvalues is particle-hole symmetric.

### 7.6.5 Topological invariant

#### 7.6.5.1 Single glide

Ref 185 introduces a $\mathbb{Z}_4$ invariant to classify strong topological phases of time-reversal invariant systems with a single glide symmetry; Ref 9 shows how to interpret this invariant in terms of Wilson loops. Here, we refine this invariant for systems with two glide symmetries.

We first summarize the relevant result from Ref 185. Consider a time reversal-invariant system with a single glide symmetry, $g_y = \{M_y|\frac{1}{2}t_y0\}$, where $t_y$ can be a fractional or integer translation. Since $g_y^2 = \{\mathcal{R}|100\}$, where $\mathcal{R}$ indicates a $2\pi$
rotation, Eq (7.6.13) dictates that \( g_{y,(k_x,k_y,k_z)}^2 = -e^{i k_z} \), where the minus sign comes because we are considering spinful systems that acquire a minus sign upon a \( 2\pi \) rotation. Hence, along the glide-invariant planes, \( k_y = 0 \) and \( k_y = \pi \), each band can be labelled by its \( g_{y,(k_x,k_y,k_z)} \) eigenvalue, \( \pm ie^{i k_z/2} \), and we say it belongs to the \( \pm \) glide sector. The \( \mathbb{Z}_4 \) invariant is defined as,

\[
\chi_y \equiv \frac{2}{\pi} \int_{-\pi}^\pi dk_z \left( \text{tr} A^I_{+,z}(\pi, \pi, k_z) - \text{tr} A^I_{+,z}(\pi, 0, k_z) \right) + \frac{1}{\pi} \int_0^\pi dk_x \int_{-\pi}^\pi dk_z \left( \text{tr} F_{+,y}(k_x, \pi, k_z) - \text{tr} F_{+,y}(k_x, 0, k_z) \right) - \frac{1}{2\pi} \int_0^\pi dk_y \int_{-\pi}^\pi dk_z \text{tr} F_x(0, k_y, k_z) \mod 4, 
\]

where \( A_{\pm,i} \equiv i \langle u^\pm | \partial_{k_i} | u^{\pm} \rangle \), \( F_{\pm} \equiv \nabla \times A_{\pm} \), the subscript \( \pm \) indicates the glide sector (when there is no subscript, both sectors are summed over), and the superscript \( I \) indicates one state in a Kramers pair. It is shown in Ref 185 that \( \chi_y \) always takes integer values. It is also gauge invariant: the first line compensates for any change of gauge implemented in the last two lines. Thus, \( \chi_y \) at least partially classifies time-reversal invariant systems with one glide. Using \( K \) theory, Ref 185 claims that it is a complete classification of strong topological phases.

Before moving to systems with two glide symmetries, it is useful to translate Eq (7.6.33) into a pictoral computation from a plot of the Wilson loop (defined in Eq (7.6.28)) eigenvalues along the line segment \( \bar{M}\bar{Y}\bar{\Gamma}\bar{X} \) (notice this is a bent line[6] consisting of three segments, not a complete loop):
1. Draw a horizontal line across the plot.

2. Count the number of times a positively-sloped band in the + sector crosses the line along the $\bar{M}\bar{Y}$ segment and subtract from it the number of times a negatively-sloped band in the + sector crosses the line along the same segment. Multiply the total by 2.

3. Repeat along the $\bar{\Gamma}\bar{X}$ segment.

4. Along the $\bar{Y}\bar{\Gamma}$ segment, count the number of times any positively-sloped band crosses the line and subtract from it the number of times a negatively sloped band crosses the line.

5. Add the numbers from the previous three steps together; taken mod 4, this sum is $\chi_y$.

An example is shown in Fig 7.4.

7.6.5.2 Two glides

We now consider systems with two glide symmetries, $g_x$ and $g_y$, which satisfy $g_x^2(\bar{k}_x,\bar{k}_y,\bar{k}_z) = -e^{ik_y}$, $g_y^2(\bar{k}_x,\bar{k}_y,\bar{k}_z) = -e^{ik_x}$. Such a system can be described by a pair of invariants $(\chi_x, \chi_y)$, where $\chi_x$ is defined by exchanging $k_x$ and $k_y$ in Eq (7.6.33). However, not all pairs are compatible: we now show that $\chi_x + \chi_y = 0 \mod 2$. The parity of $\chi_{x,y}$ is determined entirely by the result of step 4 above (because steps 2 and 3 include multiplication by 2); thus, $\chi_{x(y)} \mod 2$ is exactly the parity of the
Figure 7.4: An example to compute $\chi_y$ according to steps 1-4 in the text. The $\pm$ glide sectors are identified by solid black (dashed blue) lines for the bands with $g_y$ eigenvalue $\pm e^{i k_y/2}$ along $\tilde{M}\tilde{Y}$ and $\tilde{\Gamma}\tilde{X}$ (analogous labelling is used for the $\pm$ glide sectors of $g_x$ along $\tilde{Y}\tilde{\Gamma}$.) We now follows steps 1-4 to compute $\chi_y$: 1. Draw the red line labelled $E_1$. 2. One positively-sloped line in the $+$ sector (black solid line) crosses $E_1$ along $\tilde{M}\tilde{Y}$ and no negatively-sloped lines cross; after multiplying by 2 the total for this step is 2. 3. One positively-sloped line in the $+$ sector (black solid line) crosses $E_1$ along $\tilde{\Gamma}\tilde{M}$ and no negatively-sloped lines cross; after multiplying by 2 the total for this step is 2. 4. Along $\tilde{Y}\tilde{\Gamma}$, one line with positive slope and one line with negative slope cross $E_1$; the total for this step is zero. The total from steps 2, 3, and 4 is 4. Thus, $\chi_y = 4 \mod 4 = 0$ in this example. We could have also seen that $\chi_y = 0$ by choosing in step 1 the red horizontal line at energy $E_2$. Since no bands cross this line, steps 2-4 again shows that $\chi_y = 0$.

number of bands between $\tilde{Y}\tilde{\Gamma}(\tilde{X}\tilde{\Gamma})$ which cross the horizontal reference line drawn in step 1. The total number of Wilson bands that cross the reference line around the closed loop $\tilde{\Gamma}\tilde{X}\tilde{M}\tilde{Y}\tilde{\Gamma}$ must be even because the system is gapped and, consequently, the integral of the Berry curvature over any closed surface must be zero. But since the bands along the segment $\tilde{Y}\tilde{M}\tilde{X}$ are double-degenerate (shown in Sec 7.6.4.2), the parity of the winding number is equal to the parity of the number of bands that cross the reference line along the segment $\tilde{X}\tilde{\Gamma}\tilde{Y}$, which is exactly $\chi_x + \chi_y \mod 2$. Thus, $\chi_x + \chi_y = 0 \mod 2$, showing that there are eight topologically distinct surface phases that describe the system with two glide symmetries. The eight possible Wilson loops corresponding to the pair of invariants are shown in the main text.
Because $\chi_x + \chi_y = 0 \mod 2$, we can rewrite each pair of invariants as $(\chi_x, \chi_y) = (\chi_x, \chi_x + 1 - (-1)^{(\chi_x - \chi_y)/2})$, which shows that the eight topological phases are classified by a $\mathbb{Z}_4 \times \mathbb{Z}_2$ index, namely the $\mathbb{Z}_4$ index is given by the $\mathbb{Z}_4$ index of a single $g_x$ glide, $\chi_x$, and the $\mathbb{Z}_2$ index is $\eta_{\chi_x, \chi_y} \equiv \frac{1}{2} \left( 1 - (-1)^{(\chi_x - \chi_y)/2} \right)$. It is straightforward to check that the $\mathbb{Z}_2$ index satisfies the desired group addition:

$$
\eta_{\chi_x, \chi_y} + \eta_{\chi_x', \chi_y'} \equiv \frac{1}{2} \left( 1 - (-1)^{(\chi_x - \chi_y)/2} \right) + \frac{1}{2} \left( 1 - (-1)^{(\chi_x' - \chi_y')/2} \right)
= \frac{1}{2} \left( 1 - (-1)^{(\chi_x + \chi_x' - \chi_y + \chi_y')/2} \right) + \left( 1 - (-1)^{(\chi_x - \chi_y)/2} \right) \left( 1 - (-1)^{(\chi_x' - \chi_y')/2} \right)
= \frac{1}{2} \left( 1 - (-1)^{(\chi_x + \chi_x' - \chi_y + \chi_y')/2} \right) \mod 2 \equiv \eta_{\chi_x + \chi_x', \chi_y + \chi_y'}
\quad (7.6.34)
$$

We now consider what would happen if instead of computing $\chi_{x,y}$ in the first Brillouin zone, we looked at an adjacent Brillouin zone, shifted by $2\pi$ along the $k_x$ axis. In this case, the $g_y$ eigenvalues change sign, $\pm i e^{i k_x/2} \rightarrow \mp i e^{(i k_x + 2\pi)/2}$, while the $g_x$ eigenvalues would remain invariant. Consequently, $\chi_y \rightarrow -\chi_y$, while $\chi_x$ remains unchanged. Similarly, if we moved to a Brillouin zone shifted by $2\pi$ in the $k_y$ direction, $\chi_y$ would be unchanged, but $\chi_x \rightarrow -\chi_x$. Thus, one might worry that the $\mathbb{Z}_4$ invariant is not a robust characterization of the phase. This is not the case: while the labels depend on our choice of Brillouin zone, once that choice is made, there are always eight distinct topological phases.

As some phases depend on the odd-even choice of BZ, then not all of the insu-

302
lating phases will ordinarily be physically distinguishable. Specifically, as long as the surface remains translationally invariant, then quantities that depend on the choice of BZ, such as the odd sector of $\chi_{x,y}$, cannot be physically distinguishably. Therefore, even though $\chi_{x,y} = 1,3$ are topologically distinct phases, they will not be distinguishable in experiments such as ARPES, which preserve surface translational symmetry. However, experiments that break translational invariance by, for example, placing two samples side-by-side, can distinguish between distinct topological phases by the presence/absence of surface states at the boundary between the two samples. This effect is similar to what occurs in time-dependent adiabatic pumping cycles of topological superconducting Josephson Junctions, for which there are two distinct QSH-like phases that in practice are only distinguishable when coupled to other similar systems [252].

7.6.5.3 $\mathbb{Z}_2$ topological invariant in the presence of inversion symmetry

In the presence of inversion symmetry, $\mathcal{I}$, the $\mathbb{Z}_2$ strong topological invariant, $\nu$, is given by,

$$
\nu = \prod_{\mathbf{k}_{\text{inv}}} \xi_{\mathbf{k}_{\text{inv}}},
$$

(7.6.35)

where the product is over the eight inversion-symmetric points, $\mathbf{k}_{\text{inv}}$, and $\xi_{\mathbf{k}_{\text{inv}}}$ is the product of inversion eigenvalues of the occupied bands at $\mathbf{k}_{\text{inv}}$ that are not time-reversal partners (since time-reversal partners have the same inversion eigenvalues, there is no ambiguity in this definition.) In this section, we show that in the presence
of the two glides, \( g_x, g_y \), and inversion symmetry, Eq (7.6.35) can be simplified to only involve two points:

\[
\nu = \xi_{(0,0,0)} \xi_{(0,0,\pi)}
\]  

(7.6.36)

Without loss of generality, in this section we choose the crystal origin so that the inversion operator is symmorphic. The two glides can be expressed as \( g_x = \{ m_x | t_x 0 \} \), \( g_y = \{ m_y | 0 t_y \} \), where \( t_{x,y} = 0 \) or \( \frac{1}{2} \), depending on the space group. We do not consider translations in the \( \hat{z} \) direction since these symmetries would not be preserved by a surface parallel to the \( xy \)-plane. The operators obey the following commutation relation:

\[
\mathcal{I} g_x = g_x \mathcal{I} t - 2 t_x \hat{x} + \hat{y}
\]

(7.6.37)

and the same with \( x \leftrightarrow y \); \( t_v \) indicates a translation by \( \mathbf{v} \).

At the two points \((\pi, \pi, 0(\pi))\), which project in the surface Brillouin zone to the \( \bar{M} \) point, where a Dirac node is located, filled bands come in groups of four that are eigenstates of \( g_y \): \( \psi, g_x \psi \) and their time-reversed partners; notice \( \psi \) and \( g_x \psi \) are linearly independent and not time-reversal partners because they have different \( g_y \) eigenvalues (at the \( \bar{M} \) point, \( \{ g_x, g_y \} = 0 \)). At \((\pi, \pi, 0)\), for each eigenstate, \( \psi \), with inversion eigenvalue \( \lambda = \pm 1 \), the state \( g_x \psi \) has inversion eigenvalue

\[
\lambda e^{(-2 t_x + 1) \pi i},
\]

following Eq (7.6.37). Thus, \( \xi_{(\pi,\pi,0)} = (-e^{2 \pi i t_x})^{n_{occ}/4} \). Since the same logic holds at the \((\pi, \pi, \pi)\) point, \( \xi_{(\pi,\pi,\pi)} = (-e^{2 \pi i t_x})^{n_{occ}/4} \), as well. Since \( t_x = 0 \) or \( \frac{1}{2} \), \( \xi_{(\pi,\pi,0)} \xi_{(\pi,\pi,\pi)} = (e^{4 \pi i t_x})^{n_{occ}/4} = 1 \).
We now assume the presence of $C_{4z}$ to show that the points $(0, \pi, 0(\pi))$ and $(\pi, 0, 0(\pi))$ also contribute a factor of $+1$ to $\nu$. Since $[C_{4z}, I] = 0$, an eigenstate at $(0, \pi, 0(\pi))$ has a $C_{4z}$ partner at $(\pi, 0, 0(\pi))$ with the same inversion eigenvalues; hence the product of the inversion eigenvalues at these two points is $+1$. This proves Eq (7.6.36) in the presence of $C_{4z}$ symmetry.

We now prove Eq (7.6.36) without $C_{4z}$ symmetry using the $Z_4$ invariants, $\chi_{x,y}$. In Appendix 7.6.5.1, we proved that the two $Z_4$ invariants have the same parity: $(-1)^{\chi_x} = (-1)^{\chi_y}$. Ref 185 proves that, $(-1)^{\chi_x} = \xi(0,0,0)\xi(\pi,0,0)\xi(\pi,\pi)\xi(\pi,0,\pi)$, i.e., the $Z_2$ index of the $k_y = 0$ plane. Similarly, $(-1)^{\chi_y} = \xi(0,0,0)\xi(0,\pi,0)\xi(0,0,\pi)\xi(0,\pi,\pi)$, the $Z_2$ index of the $k_x = 0$ plane. Since these two quantities are equal, $\xi(\pi,0,0)\xi(\pi,\pi) = \xi(0,\pi,0)\xi(0,\pi,\pi)$. Hence, the inversion eigenvalues at these points contribute a (trivial) $+1$ to Eq (7.6.35). We already showed above that the two points $(\pi, \pi, 0(\pi))$ also contribute a factor of $+1$. Together, this proves Eq (7.6.36).

7.6.5.4 Mirror Chern number in Wallpaper Group $p4g$

The wallpaper group $p4g$ has $C_{4z}$ symmetry, in addition to the two glides, $g_{x,y}$. Consequently, it has the two mirror symmetries $m_{1\bar{1}0} \equiv \{M_{1\bar{1}0}|\frac{1}{2}\bar{2}0\}$ and $m_{110} \equiv \{M_{110}|\frac{1}{2}\bar{2}0\}$. These symmetries are mirrors, and not glides, because their associated translations are along the same axis that the mirror reflects over. Equivalently, for a different choice of origin, these mirrors could be written without an accompanying translation). One can define mirror Chern numbers,[201] $n_{1\bar{1}0}$ and $n_{110}$, associated
with \( m_{110} \) and \( m_{110} \), respectively.

We now show that \((-1)^{n_{110}} = (-1)^{n_{110}} = (-1)^{x_y} = (-1)^{x_y} \) (the last equality was proved in Sec 7.6.5.1.) For illustrative purposes, we focus on the mirror Chern number \( n_{110} \), associated with \( m_{110} \), which leaves the line \((k,k,k_z)\) invariant; an identical argument holds for \( n_{110} \). As shown in Ref 8,

\[
n_{110} = \frac{1}{2\pi} \int_{0}^{\pi} dk_{11} \int_{0}^{2\pi} dk_z \text{tr} \left[ F_{+,11} - F_{-,11} \right], \quad (7.6.38)
\]

where \( k_{11(11)} \equiv \frac{1}{\sqrt{2}}(k_x \pm k_y) \) and here, \( F_{\pm,11} \equiv \partial_{k_{11}} A_{\pm,z} - \partial_{k_z} A_{\pm,11} \), where \( \pm \) indicates that the trace is over bands with \( m_{110} \) eigenvalue \( \pm i \). By choosing a gauge where the eigenstates satisfy \( |u^n(k)\rangle = |u^n(k + 2\pi \hat{z})\rangle \), Eq (7.6.38) can be rewritten:

\[
n_{110} = \frac{1}{2\pi} \int_{0}^{\pi} dk_{11} \partial_{k_{11}} \text{Tr} \left[ \int_{0}^{2\pi} dk_z (A_{+,z} - A_{-,z}) \right] \\
= -\frac{i}{2\pi} \int_{0}^{\pi} dk \partial_{k_{11}} \text{Tr} \left[ \ln W_{(k,k,0)}^{+} - \ln W_{(k,k,0)}^{-} \right], \quad (7.6.39)
\]

where \( W^{\pm} \) is defined as the Wilson loop evaluated on the bands with \( m_{110} \) eigenvalue \( \pm i \). Thus, \( n_{110} \) can be evaluated from a plot of the phases of the eigenvalues of the Wilson loop \( W_{(-k,k,0)} \) along the line \( \Gamma \bar{M} \), similar to Sec 7.6.5.1:

1. Draw a horizontal reference line across the plot

2. Count the number of times a positively-sloped line in the + sector crosses
the horizontal reference line and subtract from that the number of times a negatively-sloped line in the + sector crosses the horizontal reference line

3. Repeat for the − sector

4. $n_{110}$ is equal to the result from step 2 minus the result from step 3

This is illustrated in Ref 8 and in Fig 7.5. From steps 1-4, it is evident that the parity of $n_{110}$ is equal to the parity of the number of lines crossing the horizontal reference line drawn in step 1, along the segment $\bar{\Gamma} \bar{M}$. Now consider the closed loop in the surface Brillouin zone, $\bar{\Gamma} \bar{M} \bar{X} \bar{\Gamma}$. If the Wilson loop, $W_{(k_x,k_y,0)}$ is plotted along this loop, the total number of positively-sloped bands crossing the reference line must be equal to the number of negatively-sloped bands, since the system is insulating and time-reversal invariant. Since the bands come in pairs along the line $\bar{M} \bar{X}$, the parity of the number of bands crossing the reference line along $\bar{\Gamma} \bar{M}$ is equal to the parity of the number of bands crossing the reference line along $\bar{X} \bar{\Gamma}$; the latter is equal to the parity of $\chi_y$, as derived at the end of Sec 7.6.5.1. It follows that $n_{110} = \chi_y \mod 2$, completing the proof.

Finally, we note that $n_{110} \mod 2$ is equal to the strong $\mathbb{Z}_2$ index, i.e., if $n_{110}$ is odd, the occupied bands constitute a strong topological insulator phase.

7.6.6 Tight-Binding Model and the SSH Limit

307
Figure 7.5: An example to compute $n_{110}$ according to steps 1-4 in the text. Along $\Gamma M$ the solid black (dashed blue) lines indicate the bands with $m_{110}$ eigenvalues $\pm i$. Along $MX(\bar{X}\Gamma)$ the solid black (dashed blue) lines indicate bands with $g_x(g_y)$ eigenvalue $\pm ie^{ik_x/2}(\pm ie^{ik_y/2})$. To compute steps 1-4, we need only examine the segment $\Gamma M$, along which one negatively-sloped line in the + sector and two negatively-sloped lines in the − sector cross the red horizontal reference line. Thus, the result from step 2 is -1, the result from step 3 is -2, and $n_{110} = 1$. Evaluating $\chi_x$ according to Sec 7.6.5.1 shows that $\chi_x = 1 \mod 2$, exemplifying the proof that $\chi_x = n_{110} \mod 2$.

In this section, we present a simplified tight-binding model that can realize all of the $\mathbb{Z}_4 \times \mathbb{Z}_2$ insulating phases allowed for wallpaper groups $pgg$ and $p4g$, which have perpendicular glides, $g_{x,y}$, in the $x$ and $y$ directions. For simplicity, we further specialize to systems with inversion symmetry, $I$; as shown in Sec 7.6.5.3, this simplifies the computation of the $z$-projecting Wilson loop. Inversion symmetry also implies the presence of a mirror in the $z$ direction: $I = g_x g_y m_z$. We find a fine-tuned limit in which the $\mathbb{Z}_4$ topological invariants defined in Sec 7.6.5.1 can be computed by comparing the relative values of three Su-Schrieffer-Heeger $\mathbb{Z}_2$ invariants defined by 1D models at the corners of the BZ. This limit provides an alternative way to understand the four topological phases where $\chi_x = \chi_y = 0 \mod 2$. 308
As a starting point, consider a single layer of the two-site unit cell shown in Figure 7.1. The sites, designated A and B, are related to each other by glide mirrors, \( g_{x,y} = \{M_{x,y}|\frac{1}{2}\frac{1}{2}\}\); the origin is defined to sit at an A site. An orthorhombic stack of this single layer, with no other symmetries, is in space group 32, \( Pba2 \), and its \( z \)-normal (001) surface is characterized by the two-dimensional wallpaper group, \( pgg \).

We enforce an extra symmorphic mirror, \( m_z = \{M_z|00\frac{1}{2}\}\), by adding two more sublattices, \( C \) and \( D \), sitting \( t_{z/2} \) above the \( A \) and \( B \) sites respectively; this mirror implies that the system also has inversion symmetry. The resulting system is in space group 55 \( Pbam \). In this space group, when the two layers are decoupled, each sheet is equivalent to a single layer of the two-dimensional Dirac semimetal model in Ref. 245, which possesses four-fold degeneracies at \( X \), \( Y \), and \( M \) due to the commutation relations between inversion symmetry and the glides at those TRIMs. Specifically, using the algebra from Sec 7.6.1.2, the glides anticommute with inversion at those TRIMs and \( T^2 = +1 \).

The following Hamiltonian includes all allowed in-plane hopping terms up to
second-nearest-neighbor:

\[ H_{xy}(\vec{k}) = \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [t_1 \tau^x + v_{s1} \tau^y \sigma^z] \]
\[ + \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) [v_{s1} \tau^x \mu^z \sigma^y] \]
\[ + \cos \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) [v'_{s1} \tau^x \mu^z \sigma^x] \]
\[ + \cos (k_x) t_{2x} + \cos (k_y) t_{2y} \]
\[ + \sin (k_x) [v_{s2} \tau^x \mu^z \sigma^x + v'_{s2} \mu^x \sigma^y] \]
\[ + \sin (k_y) [v''_{s2} \mu^x \sigma^x + v'''_{s2} \mu^x \sigma^y], \] (7.6.40)

where \( \tau^x \) corresponds to hopping between the A and B (or C and D) orbitals, \( \mu^x \) corresponds to hopping between the A and C (or B and D) orbitals and the \( \sigma \) Pauli matrices correspond to an on-site spin.

To further simplify, we impose \( C_{4z} \) symmetry, which is implemented by the operator, \( C_{4z} = \sqrt{i \sigma^z} f_{4z}(\vec{k}) \), where \( f_{4z}(\vec{k}) \) acts on the crystal momenta by enforcing the cyclical mapping:

\[ \sigma^x \to \sigma^y, \ \sigma^y \to -\sigma^x, \ \sigma^z \to \sigma^z \]
\[ k_x \to k_y, \ k_y \to -k_x, \ k_z \to k_z. \] (7.6.41)

With this additional symmetry, \( v_{s1} = -v'_{s1}, \ v_{s2} = -v''_{s2}, \ v'_{s2} = v'''_{s2} \) in Eq. 7.6.40 and the system is now in the higher-symmetry space group 127, \( P4/mbm \), with an
in-plane Hamiltonian up to second-nearest neighbor hopping:

\[
\mathcal{H}_{xy}(\vec{k}) = \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) \left[ t_1 \tau^x + v_{r1} \tau^y \sigma^z \right] \\
+ v_{s1} \left[ \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) \tau^x \mu^z \sigma^y \right] \\
- \cos \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) \tau^x \mu^z \sigma^x \\
+ t_2 \left[ \cos (k_x) + \cos (k_y) \right] \\
+ v_{s2} \left[ \sin (k_x) \mu^z \sigma^y \right] \\
+ v_{s2}' \left[ \sin (k_x) \tau^z \mu^z \sigma^x \right].
\]

(7.6.42)

We now add hopping in the \( z \)-direction to couple the layers. We begin with terms that do not involve the spin degree of freedom, as shown in Fig. 7.6:

\[
V_z(k_z) = \cos \left( \frac{k_z}{2} \right) u_1 \mu^x + \sin \left( \frac{k_z}{2} \right) u_2 \mu^y \\
+ \cos \left( \frac{k_z}{2} \right) \left[ \cos (k_x) + \cos (k_y) \right] v_1 \mu^x \\
+ \sin \left( \frac{k_z}{2} \right) \left[ \cos (k_x) + \cos (k_y) \right] v_2 \mu^y.
\]

(7.6.43)

The terms proportional to \( u_{1,2} \) correspond to hopping between nearest-neighbor \( A \) (\( B \)) and \( C \) (\( D \)) sites. Terms proportional to \( v_{1,2} \) originate from longer-range versions of the same type of hopping, and connect \( A \) (\( B \)) and \( C \) (\( D \)) sites separated by \( \vec{d} = \{10 \frac{1}{2} \} \) and \( \vec{d} = \{01 \frac{1}{2} \} \).
\[
\mathcal{H}_{127}(\vec{k}) = \mathcal{H}_{xy}(\vec{k}) + V_z(k_z).
\] (7.6.44)

We now consider the fine-tuned limit where \( v_{r1} = v_{s1} = 0 \); in this limit, there is no spin-orbit coupling (SOC) at \((k_x, k_y) = (\pi, 0)\) and \((0, \pi)\). In this limit, we can write down the Hamiltonian under \( \bar{X} \):

\[
\mathcal{H}^{SSH}_{\bar{X}} = \cos \left( \frac{k_z}{2} \right) u_1 \mu^x + \sin \left( \frac{k_z}{2} \right) u_2 \mu^y
\] (7.6.45)

where we have shifted the energy to make \( t_2 = 0 \) without loss of generality. We note that the \( \tau \) sublattice and \( \sigma \) spin degree of freedoms no longer play a role, and just act as additional degeneracies.

This limit places strong constraints on the Wilson loop bands: since the spins are decoupled, we can consider the spinless time reversal operator, \( \tilde{T} \), which satisfies \( \tilde{T}^2 = +1 \) and the spinless glide, \( \tilde{g}_y \), which, at the \( \bar{X} \) point, satisfies \( \tilde{g}_y^2 = -1 \). Thus, at \( \bar{X} \), \( \tilde{T} \tilde{g}_y \) is an anti-unitary operator that squares to \(-1\), enforcing that all eigenstates are doubly-degenerate, within each spin sector. Since there is no SOC, the two spin sectors are also degenerate, resulting in a four-fold degeneracy at the \( \bar{X} \) point. In addition, inversion requires that the Wilson bands are particle-hole symmetric.\[9\] Thus, our four-band model has all four Wilson bands degenerate at the \( \bar{X} \) point and, because of inversion symmetry, they are pinned to either 0 or \( \pi \).
It was shown in Sec 7.6.4.3 that all four Wilson bands are degenerate at the $\bar{M}$ point, as well, and thus are also pinned to either 0 or $\pi$. Since the Wilson bands must continuously connect the bands at $\bar{X}$ to the bands at $\bar{M}$, there is a $\mathbb{Z}_2$ invariant that characterizes the possible connectivities for fixed band inversion at $\bar{\Gamma}$:

$$\chi = 2 \left( \left\lfloor \frac{1}{\pi} (\theta(\bar{M}) - \theta(\bar{X})) \right\rfloor \mod 2 \right)$$  \hspace{1cm} (7.6.46)

One of these connectivities is a trivial phase and the other is the topological Dirac insulating phase. As long as the system is QSH-trivial and diagonal symmorphic mirror Chern-trivial, then the Wilson loop eigenvalues are generically unpinned at $\bar{\Gamma}$ and along all low symmetry lines. Therefore, in this particular model of SG 127, all of the possible crystalline connectivities for the path $\bar{\Gamma}\bar{X}\bar{M}\bar{X}'$ are entirely determined by how the eigenvalues are pinned at $\bar{X}$ and $\bar{M}$.

This limit can also be described by two, doubly-degenerate Su-Schrieffer-Heeger (SSH) chains, where the edge state of one chain is the projection of the Hamiltonian onto $\bar{X}$ and the other is the projection onto $\bar{M}$. The relative values of the $u_{1,2}$ and $v_{1,2}$, which parameterize hopping in the $z$-direction, correspond to the two choices of dimerization for each SSH chain. For each of these two chains, there is a $\mathbb{Z}_2$ polarization, $\theta = 0, \pi$, which directly corresponds to the Wilson phases at those surface TRIMs, and the overall bulk topology for these crystalline phases is given by the $\mathbb{Z}_2$ relative polarization between the two SSH models.

However, within each chain, there is an additional degeneracy because the orig-
inal SSH model only has two occupied bands. Thus, each SSH-like chain in our model consists of two identical uncoupled Hamiltonians of the original SSH model. For the chain which projects to $\bar{M}$, the four-fold surface degeneracy prevents the two Hamiltonians from coupling. However, for the chain projecting to $\bar{X}$, the two SSH Hamiltonians are only prevented from coupling in the limit that there is no SOC coupling at any bulk $k$-point projecting to $\bar{X}$. As symmetry-allowed SOC terms are turned on, a real system will escape this limit, and the two copies of the SSH Hamiltonian at $\bar{X}$ will couple and their surface states will gap into pairs.

7.6.6.2 Beyond the SSH Limit

Generically, all symmetry-allowed hopping terms will be present, including $v_{r1}$, $v_{s1}$, and the other $z$-direction hopping terms. In this section, we will examine how this affects the SSH-model definition of crystalline invariants.

The line that projects to $\bar{M}$ continues to be described by a double-degenerate SSH chain even after generic terms are added, as it still hosts a four-fold degenerate surface state with a $\mathbb{Z}_2$ polarization. As states at $\bar{M}$ are four-fold degenerate due to surface wallpaper symmetries, the Wilson phases $\theta(\bar{M})$ must still be either 0 or $\pi$ as long as there is bulk inversion symmetry. Though this doesn’t guarantee a topological Wilson loop connectivity by itself, in the limit of weak spin-orbit interaction, the presence of a band inversion at an $\bar{M}$-projecting TRIM nevertheless still results, for weak band inversion, in the presence of topological Dirac point or line
nodes. The properties of these line nodes and their relationship to nonsymmorphic symmetries are discussed are space-group dependent, and in general go beyond the focus of this chapter.

At the TRIMs which project onto $\bar{X}$, the immediate consequences of allowing nonzero values of $v_{r1}$ and $v_{s1}$ are to couple the two copies of the SSH Hamiltonians under $\bar{X}$ and gap out their surface states. As states at $\bar{X}$ are only generically two-fold degenerate, the presence of additional SOC terms breaks the artificial symmetries $\tilde{g}_y$ and $\tilde{T}$ and gaps the states into the two ends of an hourglass. Nevertheless, as pictured in Fig. 7.8, this hourglass along $\bar{\Gamma}\bar{X}$ is still characterized by a $\mathbb{Z}_2$ invariant that characterizes whether it is centered about a Wilson phase of 0 or $\pi$. Therefore, as long as there are no additional band inversions, then as the connectivity remains unchanged, away from the SSH limit there still is an overall $\mathbb{Z}_2$ quantity that characterizes the crystalline Wilson connectivity. However, as the phase of the hourglass center can be moved by any band inversion on the plane which projects to $\bar{\Gamma}\bar{X}$, then we find that this $\mathbb{Z}_2$ invariant is no longer just a property of the TRIMs, and so for a real double-glide system, the Wilson loop remains the only generic method for evaluating the bulk topology.

7.6.6.3 Broken $C_{4z}$ Phases

Additional Wilson band topologies are possible in systems without $C_{4z}$ symmetry, whose surfaces are described by the wallpaper group $pgg$. We break $C_{4z}$ symmetry
in the tight-binding model by adding another interlayer hopping term:

\[ V_{C4} = v_{C4} \mu^x \cos (k_y) \cos \left( \frac{k_z}{2} \right) \]  

(7.6.47)

The resulting system is now in SG 55. Without \( C_{4z} \) symmetry, the SSH polarizations at \( \bar{X} \) and \( \bar{Y} \) can now differ, leading us to define a second crystalline invariant for the independent \( y \) direction:

\[ \chi_{x,y} = 2 \left[ \frac{1}{\pi} \left( \theta(\bar{M}) - \theta(\bar{Y}, \bar{X}) \right) \right] \text{ mod } 2 \]  

(7.6.48)

The reason that \( \chi_{x,y} \) is determined by \( \theta(\bar{Y}, \bar{X}) \), as opposed to the opposite order of indices, is because \( g_y \) enforces a four-fold degeneracy at \( \bar{X} \), as explained in Sec 7.6.6.1. Thus, \( \chi_{x,y} \) is determined by \( g_{x,y} \), consistent with the notation in Sec 7.6.5.2.

If the polarization at \( \bar{X} \) differs from that at \( \bar{Y} \) and \( \bar{M} \), the system can display a single four-fold point at \( \bar{X} \). As more symmetry-allowed terms are added, the states at \( \bar{X} \) will couple and the four-band crossing will open up into an hourglass along \( \bar{\Gamma} \bar{X} \). Nevertheless, as long as the bulk symmetries and band inversions are unchanged, the Wilson connectivity will be preserved and the \( C_{4z} \)-broken SSH phase will evolve into a crystalline hourglass phase. An observation of the allowed Wilson band connectivities with broken \( C_{4z} \) symmetry confirms in fact that these two phases (hourglasses along \( \bar{\Gamma} \bar{X} \) or along \( \bar{\Gamma} \bar{Y} \)) are the only two allowed topological crystalline connectivities which fundamentally violate \( C_{4z} \). The \( (\chi_x, \chi_y) = (0, 2) \) phase is
demonstrated in our tight binding model in Figure 7.9.

If symmetry-allowed terms are made larger, other band inversions may occur and $\chi_{x/y}$ may eventually change. However, the resulting phases, if QSH-trivial, will still ultimately be tunable back to an SSH limit. Therefore the SSH limit can be considered as a parent phase to all four possible $\chi_{x,y} = 0, 2$ crystalline insulating phases.

7.6.6.4 Strong Topological Insulating Phases

Away from the SSH limit, but preserving $C_{4z}$ symmetry such that the system is in SG 127, as shown in Sec. 7.6.5.3, a band inversion about a TRIM which projects to $\bar{\Gamma}$ can flip the product of parity eigenvalues and induce a strong topological insulating phase. In practice, this band inversion can be accomplished in our tight-binding model by adding the term:

$$V_{TI} = v_{TI} \tau^y \mu^z \sigma^z \cos \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) \cos \left( \frac{k_z}{2} \right)$$  \hspace{1cm} (7.6.49)

to the Hamiltonian in Eq. 7.6.44. Observing the glide-sector-resolved Wilson loop in Fig. 7.10(b), we observe that this demonstrated double-glide spin hall phase is characterized by $\chi_x = \chi_y = 1$ or 3, depending on our choice of labeling.
Figure 7.6: The $xz$-plane consisting of $A$ and $C$ sites of the tetragonal lattice for our tight-binding model of space group 127, with lattice spacings $a_{x/z}$ (there is a distinct $xz$-plane consisting of $B$ and $D$ sites that is not visible in this slice). The chains in the $z$-direction can be considered Su-Schrieffer-Heeger (SSH) chains, with hoppings proportional to $u_{1/2}$ dimerizing chains in a strictly $z$-dependent way and hoppings proportional to $v_{1/2}$ coupling sites one lattice spacing $a_x$ (or $a_y$) over so as to introduce $xy$-dependence and allow in $k$-space for terms which manifest at different TRIMs to be tuned independently.
Figure 7.7: Energy bands and \( z \)-projection Wilson bands for the SSH limit of the tight-binding model for SG 127 in Eq. 7.6.44, with the filling chosen such that the bottom four bands are occupied. Bands (a) and Wilson bands (b) display the trivial connectivity \( \chi = 0 \) when the polarization invariants at \( \bar{X} \) and \( \bar{M} \) are the same, and here were obtained using \( t_1 = 1, t_2 = 0.5, v_{s2} = -0.2, v_{s2}' = 0.15, u_1 = 0.25, u_2 = 0.45, v_{r1} = v_{s1} = u_3 = u_4 = 0 \). When the polarization invariants at \( \bar{M} \) and \( \bar{X} \) differ, which can be induced by a band inversion about \( \bar{M} \) (c), \( \chi = 2 \) and the Wilson spectrum is nontrivially connected (d). This SSH limit of the topological Dirac insulating phase in SG 127 was obtained using Eq. 7.6.44 with \( t_1 = 1, t_2 = 0.5, v_{s2} = -0.2, v_{s2}' = 0.15, u_1 = 0.85, u_2 = 1.3, u_3 = 3, v_{r1} = v_{s1} = u_4 = 0 \).
Figure 7.8: Bulk bands (a,c) and Wilson bands (b,d) for the tight-binding model (7.6.44) away from the SSH limit. The bands along $\bar{\Gamma}\bar{X}$ open up into hourglasses and the SSH edge states at $\bar{X}$ couple and gap out. For the trivial phase in panel (a), the bottom four bands approach the top four very closely in a few places, but there remains a consistent gap such that the four-band Wilson matrix is well-defined for the whole $z$-surface BZ. Occasionally, an accidental extra symmetry of the tight-binding parameters induces a four-fold degeneracy in the Wilson bands at $\bar{\Gamma}$ in this model (d). These figures were obtained by tuning $v_{r1} \to 0.55$, $v_{s1} \to 0.4$ from the values used in Fig. 7.7 for each phase.
Figure 7.9: Bulk bands (a) and Wilson bands (b) for the broken-$C_{4z}$ crystalline phase labelled by $(\chi_x, \chi_y) = (0, 2)$, realized by the tight-binding model of Eq (7.6.44). In this phase, the hourglass along $Y\Gamma$ is sharply distorted and centered around $\pi$. As occurred for the topological Dirac insulating phase in Fig. 7.8, an accidental extra symmetry of the choice of tight binding parameters can lead to a four-fold Wilson band degeneracy at $\Gamma$ (b). The picture was obtained by using the following parameters: $t_1 = 1, v_{r_1} = 0.55, v_{s_1} = 0.4, t_2 = 0.5, v_{s_2} = -0.2, v'_{s_2} = 0.35, u_1 = 0.85, u_2 = 1.3, u_3 = 3, u_4 = 4$, and $v_{C4} = 1.$
Figure 7.10: Bulk bands (a) and Wilson bands (b) for one of the double-glide QSH phases. This phase can be obtained by adding the term $V_{TI}$ in Eq. 7.6.49 to the Hamiltonian in Eq. 7.6.44 away from the SSH limit. Bands for this figure were generated using $t_1 = 1$, $v_{r1} = 0.3$, $v_{s1} = 0.25$, $t_2 = 1.5$, $v_{s2} = -0.2$, $v'_{s2} = 0.15$, $u_1 = 0.5$, $u_2 = 2$, $u_3 = u_4 = 0$, and $v_{TI} = 0.4$. 

322
Chapter 8

Filling-Enforced Magnetic Dirac Semimetals in Two Dimensions

8.1 Abstract

Filling-enforced Dirac semimetals, or those required at specific fillings by the combination of crystalline and time-reversal symmetries, have been proposed and discovered in numerous materials. However, Dirac points in these materials are not generally robust against breaking or modifying time-reversal symmetry. We present a new class of two-dimensional Dirac semimetal protected by the combination of crystal symmetries and a special, antiferromagnetic time-reversal symmetry. Systems in this class of magnetic layer groups, while having broken time-reversal symme-
try, still respect the operation of time-reversal followed by a half-lattice translation. In contrast to 2D time-reversal-symmetric Dirac semimetal phases, this magnetic Dirac phase is capable of hosting just a single isolated Dirac point at the Fermi level, one that can be stabilized solely by symmorphic crystal symmetries. We find that this Dirac point represents a new quantum critical point, and lives at the boundary between Chern insulating, antiferromagnetic topological crystalline insulating, and trivial insulating phases. We present density functional theoretic calculations which demonstrate the presence of this 2D magnetic Dirac semimetallic phase in FeSe monolayers and discuss the implications for engineering quantum phase transitions in these materials. *This chapter originally appeared as an online preprint by Steve M. Young and Benjamin J. Wieder on the arXiv in 2016 [243].*

### 8.2 Introduction

The prediction, discovery, and study of topological insulators has dramatically increased interest in topological phases of matter in general. Recently, different classes of metallic and semimetallic phases have been described and investigated; these include phases with Dirac, Weyl, Double Dirac, and Spin-1 Weyl fermions and line nodes at or near the Fermi energy. A number of variations have been predicted, and in some cases observed, in real materials [16, 24, 27, 30, 79, 95, 131, 134, 135, 137, 188, 209, 212, 213, 219, 224, 244].
In these semimetallic phases, the nodal features are stabilized by the combination of time-reversal symmetry and spatial symmetries. In particular, for the phases with nonsymmorphic spatial operations, or those symmetric under the combination of a point group operation and a fractional lattice translation, certain nodal features are always present at space-group-specific fillings [166, 216, 221]. These semimetals, known as “filling-enforced semimetals,” are prevented from being insulators at these fillings by the combination of Kramers’ theorem and nonsymmorphic symmetries, and therefore display bands inseparably tangled together in space-group-specific numbers. For example, for the simple 2D four-band models which we previously presented in Ref. 245, glides and two-fold screws forced bands to tangle together in groups of 4 such that at filling $\nu = 2$, the system always displayed Weyl or Dirac points.

In this letter, we present the first examples of filling-enforced Dirac semimetals in systems with magnetic symmetries. We find that the combination of three-dimensional layer group crystal symmetries with an antiferromagnetic time-reversal symmetry protects a single bulk Dirac point in a two-dimensional crystal, and we present four-band tight-binding models demonstrating this physics. Unlike in the Dirac semimetals with time-reversal-symmetry, this single Dirac point is permitted to exist as the only feature at the Fermi energy. Furthermore, unlike the antiferromagnetic Dirac points in Ref 198, which are topological objects created through band-inversion transitions, this 2D magnetic Dirac point is filling-enforced: it cannot be gapped without lowering the symmetry of the particular magnetic layer.
This single magnetic Dirac point, like its time-reversal-symmetric relative, represents the quantum critical point between topologically distinct insulating phases. We find that for bulk perturbations which preserve the antiferromagnetic time-reversal operation, the magnetic Dirac semimetal sits at the phase transition between a trivial insulator and a Chern-trivial antiferromagnetic topological crystalline insulator. Perturbations which break antiferromagnetic time-reversal gap to Chern insulators with winding $C = \pm 1$.

Finally, we present density functional theoretic (DFT) calculations which demonstrate the presence of this magnetic Dirac semimetal phase in FeSe monolayers, and discuss the implications for engineering topological phase transitions in these magnetic Dirac semimetals.

### 8.3 Magnetic Tight-Binding Models

At the $\mathbf{k} \cdot \mathbf{p}$ level, a four-fold point degeneracy may be protected by two spatial operations $A$ and $B$ and an antiunitary operation $\bar{T}$, where we may represent $A$, $B$, and $\bar{T}$ such that

$$\{A, B\} = [A, \bar{T}] = [B, \bar{T}] = 0, \quad A^2 = \pm B^2 = -\bar{T}^2 = +1 \quad \text{(8.3.1)}$$
Figure 8.1: (a) The lattice with $I, \{M \mid 0 \frac{1}{2}\}$, and $\bar{T} = \{T \mid \frac{1}{2} \frac{1}{2}\}$ with spins along $\pm \hat{y}$. Red and green indicate sites above and below the plane. (b) The band structure of the system generated by the tight-binding model of Eq. 8.3.2. Bands are two-fold-degenerate by the combination of $I$ and $\bar{T}$. Pictured are the top four bands of an eight-band model, which are split from the bottom bands by a very large antiferromagnetic interaction. The symmetries of this magnetic layer group necessitate that groups of four bands meet in Dirac points at the $M$ point for fillings $\nu \in 4\mathbb{Z} + 2$.

When $\bar{T}$ is plain time-reversal symmetry $T$, the above relations may only be satisfied if at least one of $A$ or $B$ is a two-fold non-symmorphic operation [221]. However, if $\bar{T} = \{T | t\}$ where $t$ is a fractional translation, then at $\bar{T}$-invariant $k$ points the commutation relations between $\bar{T}$ and spatial symmetries may be altered. We find that for some magnetic systems, this algebra can conversely be satisfied entirely using symmorphic symmetries.

The presence of a $\bar{T}$ symmetry with a half-lattice translation implies states on different sublattices are related by time-reversal, like in an antiferromagnet. To construct a model, we first consider systems with four sublattices of $s$-orbitals for
a total of eight bands. We then turn on an antiferromagnetic potential, assumed to be much stronger than other hopping and energy terms, such that the system is split into two effectively four-band systems, each with one spin per sublattice. The upper subsystem is therefore comprised of two pairs of sublattices A/B. Each pair individually respects \( T \), and the two pairs are related to one another by additional spatial symmetries, as shown in Fig. 8.1(a), for which \( t = \left( \frac{1}{2} \frac{1}{2} \right) \) and the additional symmetries are inversion \( I \) and glide reflection \( M_z \). Representing the A/B degrees of freedom by \( \sigma \) and the prime/nonprime degrees of freedom by \( \tau \), the \( \mathbf{k} \cdot \mathbf{p} \) model of the M point reads:

\[
\mathcal{I} = i\tau_y, M_z = i\tau_x\sigma_y, T = i\tau_z\sigma_y K
\]

\[
H_M = \left[ t_0\tau_x + \left( t_2^{SO} + t_3^{SO} \right) \tau_z\sigma_x + \left( t_3^{SO} + t_4^{SO} \right) \tau_z\sigma_x \right] k_x
\]

\[
- \left[ \left( t_2^{SO} - t_3^{SO} \right) \tau_z\sigma_z + \left( t_3^{SO} - t_4^{SO} \right) \tau_z\sigma_x \right] k_y
\]

and can be generated by the tight-binding model
\[ \mathcal{H} = t_0 \cos \left( \frac{k_x}{2} \right) \tau_x \]

\[ + \left[ t_1^{SO} \sin (k_x - k_y) + t_2^{SO} \sin (k_x + k_y) \right] \tau_z \sigma_z \]

\[ + \left[ t_3^{SO} \sin \left( \frac{k_x - k_y}{2} \right) + t_4^{SO} \sin \left( \frac{k_x + k_y}{2} \right) \right] \tau_z \sigma_x \]

(8.3.2)

If these two spatial symmetries were combined with regular time-reversal-symmetry \( \mathcal{T} \), Dirac points at M and Y would result. However in the little group at Y under \( \bar{\mathcal{T}} \), the translation \( \mathbf{t} \) anticommutes with both spatial operations, and no Dirac point results.

In the \( \mathbf{k} \cdot \mathbf{p} \) theory, five matrices preserve \( \bar{\mathcal{T}} \) while breaking one of the spatial symmetries: \( \tau_z, \tau_y, \tau_x \sigma_x, \tau_x \sigma_y, \text{ and } \tau_x \sigma_z \). Adding mass terms proportional to these matrices results in either insulating or Weyl semimetal phases, depending on the band ordering elsewhere in the BZ. Unlike the with time-reversal-symmetric Dirac semimetals, the resulting gapped phases in these systems cannot be evaluated by a \( \mathbb{Z}_2 \) Quantum-Spin-Hall (QSH) invariant. Furthermore, as \( \bar{\mathcal{T}}^2 = -1 \) on only a line in the bulk BZ, the system also cannot realize the inherently 3D antiferromagnetic topological insulating phase described by Mong, Essin, and Moore in Ref. 147. However, we find that this does not exclude the presence of 2D topological magnetic \textit{crystalline} phases, or those surface-protected by \( \bar{\mathcal{T}} \).

Consider the (11), (1\( \bar{1} \)), (\( \bar{1} \)1), and (\( \bar{1} \\bar{1} \)) edges, which preserve \( \bar{\mathcal{T}} \). While one
Figure 8.2: For the tight-binding model in Eq. 8.3.2, introducing an asymmetry in the interaction between $\Lambda/\Lambda'$ and $B/B'$ sites may result in edge states on $\mathcal{T}$-preserving surfaces. Pictured above is the (11) edge of a ribbon for different signs of the $M_z$-breaking term $\tau_y$ in the $\mathbf{k} \cdot \mathbf{p}$. The edge shown in (c) and represented by a red line in (a) and (b) above hosts surface states as shown in the inset band structure. The edge in (d), represented by a black line in (a) and (b), is fully gapped. Flipping the sign of $\tau_y$ is equivalent to applying $C_{2z}$ rotation, which exchanges the two crystalline phases.
Figure 8.3: (a) Perturbations corresponding to $\tau_x \sigma_x$ (along with $\tau_x \sigma_y$ and $\tau_x \sigma_z$) result in nodal phases (left) or bulk gapped phases (right), depending on perturbation strength. These cases are associated with dimerizations of the lattice, similar to what’s shown in Fig. 8.2, and may produce edge states in the same fashion (b). $\tau_z$ represents a staggered on-site potential and leads to a pair of Weyl points for small magnitudes (left), two pairs as the magnitude increases (center), and, ultimately, an insulating phase once the Weyl points annihilate (right), but never produces edge states independent of termination. (c) The chiral edge states resulting from breaking $\overline{T}$ but preserving the spatial symmetries; left and right moving states sit on opposite edges and connect the valence and bulk manifolds, and are associated with $|C| = 1$. (d) Band structure of the (10) edge of the $\overline{T}$-bulk-preserving perturbed system in Fig 8.2. This edge breaks $\overline{T}$ and hosts a single, directional trivial edge state, indicating that the $\overline{T}$-preserving bulk-insulating phases are Chern-trivial $C = 0$. 
surface Time-Reversal-Invariant-Momentum (TRIM), \( \Gamma \), has a Kramers degeneracy from \( \mathcal{T}^2 = -1 \), the other TRIM, \( Z \), does not. Including a distortion that produces the mass term \( \tau_y \) results in a bulk-insulating phase, and for appropriately chosen terminations, edge states which resemble QSH edges appear in the gap, with a linearly dispersive Kramers degeneracy forming at \( \Gamma \) as shown Fig. 8.2(c). However, at \( \bar{Z} \), Kramers’ theorem is not enforced, since \( \mathcal{T}^2 = +1 \), and the singly degenerate bands are free to move if not pinned to the bulk, and the system may fully gap as shown in Fig. 8.2(d). We find that the \( \mathcal{T} \)-preserving gapped system behaves like the Su-Schrieffer-Heeger model: \( \tau_y \) effectively dimerizes the A and B sublattices, leaving an edge state on unpaired terminations. Changing the sign of \( \tau_y \) causes dimers to switch partners, converting edge states between paired and unpaired (Figs. 8.2(a) and 8.2(b)). The terms \( \tau_x \sigma_x \), \( \tau_x \sigma_y \), and \( \tau_x \sigma_z \) also correspond to dimerizing distortions, and produce the same behavior as \( \tau_y \). Small perturbations split the Dirac point into Weyl nodes (or a nodal loop for \( \tau_x \sigma_y \), which preserves \( M_z \)), however, strong perturbations push the nodal features away from \( \bar{Z} \) until they meet and annihilate, resulting in a bulk-insulating phase with termination-dependent edge states (Fig. 8.3(a)). Conversely, \( \tau_z \) corresponds to a staggered on-site potential and, while it may generate Weyl semimetal phases, it never produces edge states, regardless of termination (Fig. 8.3(b)). In Fig. 8.3(d), we examine the \( \mathcal{T} \)-broken, low-symmetry (10) edge. While it hosts chiral edge modes for a \( \mathcal{T} \)-preserving bulk insulator, these edge modes do not connect the conduction and valence bands, and can be pushed into the bulk bands without closing the bulk gap, reflecting a Chern-trivial (\( C = 0 \))
bulk topology.

The magnetic Dirac point can also be gapped by $\tilde{T}$-breaking terms. We show in Fig 8.3(c) that applying a $\sigma_y$ term at $M$, which preserves both spatial symmetries, results in the development of a single topological chiral mode on each edge. From this we can infer that the $\tilde{T}$-broken system is Chern insulating with winding $|C| = 1$.

We may construct a similar system using only symmorphic symmetries $C_{2x}$ and $C_{2y}$ (Fig. 8.4). We note that as $C_{2x/y}$ are both two-fold and symmorphic, they would not ordinarily protect Dirac points in a time-reversal-symmetric system. [245]. However, with the antiferromagnetic $\tilde{T}$-symmetry, protection of Dirac points by symmorphic operations is conversely allowed. The translation $t$ anticommutes rather than commutes with both spatial operations at the $M$ point, converting the $k \cdot p$ theory into one that satisfies the algebra described in Eq. 8.3.1.

Its $k \cdot p$ theory looks like

$$C_{2y} = i\tau_y, C_{2x} = i\tau_x\sigma_y, \tilde{T} = i\tau_z\sigma_y K$$

$$H_M = [t_0\tau_x + t_1^{SO}\tau_z\sigma_z + t_2^{SO}\tau_z\sigma_x] k_x$$
$$+ [t_1^{SO}\sigma_z + t_2^{SO}\sigma_x + t_3^{SO}\tau_y\sigma_y] k_y$$

333
Figure 8.4: The lattice with $C_{2x}$, $C_{2y}$, and $\tilde{\mathcal{T}} = \{T|\frac{1}{2}\frac{1}{2}\}$. Magnetic moments are along $\pm \hat{y}$. The red and green sites are above and below the plane, respectively; the open-circle site is gray here to indicate that it is in the plane. The symmetries of this magnetic layer group require that bands, while singly degenerate, still group together in multiples of 4 and meet in Dirac points at $M$. Systems in this magnetic layer group are therefore filling-enforced magnetic Dirac semimetals at fillings $\nu \in 4\mathbb{Z} + 2$. 
with a tight-binding model

\[ \mathcal{H} = t_0 \cos \left( \frac{k_x}{2} \right) \tau_x + t_3^{SO} \cos \left( \frac{k_y}{2} \right) \tau_y \sigma_y \]

\[ + t_1^{SO} \left[ \sin (k_x) \cos (k_y) \tau_z \sigma_z + \sin (k_y) \cos (k_x) \sigma_z \right] \]

\[ + t_2^{SO} \left[ \sin \left( \frac{k_y}{2} \right) \cos \left( \frac{k_x}{2} \right) \tau_z \sigma_x \
+ \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) \sigma_x \right] \]

(8.3.3)

As before, \( \tau_z \) corresponds to an on-site potential breaking the symmetry between the A and B sublattices, and \( \tau_y, \tau_z \sigma_x, \tau_z \sigma_y, \) and \( \tau_z \sigma_z \) dimerize the A and B sublattices and produce similar edge states. In this case, \( \tau_z \) gaps the system directly, without an intermediate Weyl semimetal phase (Fig. 8.5(a)), whereas the dimerizing terms all produce intermediate Weyl semimetal phases (Fig. 8.5(b)). For this system as well, breaking \( \mathcal{T} \) results in \( |C| = 1 \) chiral edge states (Fig. 8.5(c)).

We note that for both magnetic Dirac systems, fillings \( \nu \in 4\mathbb{Z} + 2 \) are required.
for the Fermi energy to lie at the Dirac point. For the first model presented, the presence of multiple nonsymmorphic symmetries disallows fillings of $\nu = 2, 6$, as they would imply atoms with fractional numbers of electrons. However, derived phases for which one of the nonsymmorphic symmetries is broken are still achievable. Appropriately chosen adatoms or substrates may be able to dope the system while only weakly perturbing it, maintaining an approximate Dirac cone.

In the magnetic layer group of the second model, it is possible for pairs of sublattices to coincide, such that only two sites are necessary. In such a two-site system, the Dirac point would be allowed to sit at the Fermi energy without the distribution of electrons violating crystal symmetries. However, in practice, constructing a tight-binding model for such a system requires a more complicated pattern of magnetic ordering.

8.4 Materials Realization

As an example, we consider the iron-based superconductors. The iron pnictides – and FeSe – are comprised of layers of iron arsenide or iron selenide in the antilitharge structure [90]. Recently, monolayers of FeSe have been synthesized and investigated [68, 133]. One possible ordering of the magnetic moments takes a striped pattern (Fig. 8.6(a)). This case is represented by the first model considered above (Eq. 8.3.2), with additional symmetry such that $t_1^{SO} = t_2^{SO}$ and $t_3^{SO} = t_4^{SO}$. 

336
Figure 8.6: (a) The structure of an FeSe monolayer. The iron atoms (dark gray) form a planar square lattice, while the selenium atoms sit above and below the plane, so that the iron atoms are tetrahedrally coordinated. Magnetic moments are shown for the striped ordering phase, and are represented by the colored arrows. (b) The band structure of the striped phase of FeSe. Below the Fermi energy, the valence bands form a Dirac point at M that splits weakly along the M-X line. The splitting is due to spin-orbit interaction and its weakness is a consequence of the bands comprising primarily iron d-orbitals.

The band structure of FeSe obtained using DFT is shown in Fig. 8.6, with calculations performed using QUANTUM ESPRESSO with norm-conserving pseudopotentials generated using OPIUM [173, 175] at the level of PBE. An energy cutoff of 50Ry was used, with a $24 \times 24 \times 1$ k-point grid and 15Å of vacuum. Within the valence bands an apparent line node is visible; closer inspection reveals weak spin-orbit splitting at X, leaving a Dirac point at M as predicted.

As discussed the filling must be reduced to position the Fermi energy at the Dirac point which in this case will necessarily break the symmetry. This could potentially be achieved by using monolayers of an iron pnictide system with intercalated species on lattices that produce the correct filling.
8.5 Discussion

We have described a class of magnetic Dirac points protected by modifying time-reversal symmetry to include a fractional translation. This translation results in commutation relations with the spatial symmetries different from those in ordinary time-reversal-symmetric crystals, allowing for Fermi surfaces consisting of single Dirac points, and removing the requirement of nonsymmorphic spatial operations. Both topologically nontrivial magnetic crystalline insulating and Chern insulating phases are easily accessible from this magnetic Dirac phase by breaking symmetries. The dimerizations required to gap into the $\mathcal{T}$-preserving phases can, in general, be achieved by applying 11-direction-strain, and provide a route towards strain-engineering broken-time-reversal quantum phase transitions.

Finally, it is worth noting that this system circumvents the Dirac fermion doubling theorem for time-reversal-symmetric Dirac semimetals. In those systems, single Dirac points are prevented from being stabilized in 2D bulk crystals by the presence of additional Dirac or Weyl features. This presence of these additional nodal features at the Fermi energy prevents the nearby QSH and trivial insulating phases from being related to each other by a crystal symmetry operation [245]. Though the $\mathcal{T}$-preserving gapped phases in our systems seem to violate this doubling theorem, they are actually unrelated. The gapped phases in these magnetic Dirac systems are topological crystalline phases: or phases preserved by time-reversal and a surface-specific spatial operation, here the combined operation of time-reversal
and a diagonal half-lattice translation. The two classes of antiferromagnetic topo-
logical crystalline insulating phases in Fig. 8.2 are Chern-trivial and related to each
other by a $C_2$ operation, such that only crystalline invariants are exchanged under
spatial operations and the overall bulk topology remains unaffected. In fact, one
may instead consider the magnetic Dirac point presented here as the symmetry-
pinned combination of two, twofold-degenerate quantum Hall transitions. In that
sense, this Dirac point also successfully avoids the two-dimensional parity anomaly
addressed by Haldane in Ref. 80.

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duced in this chapter, a similar magnetic semimetal was presented in Ref. 210.
Chapter 9

Future Directions

In this final section, I provide a bit of perspective on the work presented in this thesis as it pertains to potential future research directions. For the most immediate future, I probably won’t directly build off of the transport papers highlighted in Chapters 2 and 3, unless I make a pivot back to studying Majorana fermion detection or take up numerical analysis of transport in disordered graphene along the lines of Ref. 1.

One outstanding question that I could answer through transport considerations is the role of disorder in crystalline semimetals and topological crystalline insulators. As those systems are heavily reliant on a sense of “exact” crystal symmetry, a reasonable place to start would be calculating the response of topological crystalline materials as functions of disorder strength and in different disorder ensembles, such as was done for Weyl semimetals in Ref. 179.
Currently though, my research interests lie firmly in exhausting the single-particle (or mean-field) nodal and topological systems minimally predicted by symmetry considerations. Building on the results presented in Chapters 5, 6, 7, and 8, I hope to at the very least find new Dirac and exotic unconventional fermions in systems with broken $\mathcal{I}$ or $\mathcal{T}$ symmetries, with the most obvious route again being a consideration of irreducible representations and point group symmetries. With the discovery of each of these new bulk fermions, there exists the chance for improved detection of topological physics (such as Fermi arcs) and the promise for new strain-engineered quantum phase transitions like those in Chapters 5, 7, and 8. Furthermore, there does not currently exist a complete formulation of minimal insulating filling for systems with broken $\mathcal{T}$-symmetry or time-dependence. It seems quite possible that a flat-manifold-based formulation might be achievable in time-cycle floquet or time-crystal systems [227, 259], and that it could be used to find new time-cycle semimetals [23, 211] and characterize topological quantum critical points in time-cycle systems [36, 162].

Finally, as a bit of a stretch goal, it would be interesting to study the role of crystal symmetries in interacting problems. As shown in Chapter 5, it is an open question as to whether the platycosm formulation of minimal insulating filling is truly insufficient for 10 of the 230 space groups, or whether interactions can open up symmetry-preserving gaps in those systems. There is also the possibility that a consideration of crystal symmetries and time-reversal on the phonon spectra of superconductors could be used to successfully predict new superconducting materials.
including definitive experimental realizations of topological superconductivity.

Whether or not I get to continue working in this field and address some of these problems, the last 5 years of study under Professor Kane comprise the most rewarding and enlightening time of my life. The symmetry and topology considerations presented in this thesis are the direct result of me absorbing some small sliver of Charlie’s superlative physical intuition, and whatever problems I go on to address, I hope that my work will continue to bear hallmarks of my time at Penn.
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