TOPOLOGICAL SEMIMETALS AND NODAL SUPERCONDUCTORS

BY

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DISSERTATION

Submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Physics in the Graduate College of the University of Illinois at Urbana-Champaign, 2015

Urbana, Illinois

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Abstract

Besides topological band insulators, which have a full bulk gap, there are also gapless phases of matter that belong to the broad class of topological materials, such as topological semimetals and nodal superconductors. We systematically study these gapless topological phases described by the Bloch and Bogoliubov-de Gennes Hamiltonians. We discuss a generalized bulk-boundary correspondence, which relates the topological properties in the bulk of gapless topological phases and the protected zero-energy states at the boundary. We study examples of gapless topological phases, focusing in particular on nodal superconductors, such as nodal noncentrosymmetric superconductors (NCSs). We compute the surface density of states of nodal NCSs and interpret experimental measurements of surface states. In addition, we investigate Majorana vortex-bound states in both nodal and fully gapped NCSs using numerical and analytical methods. We show that different topological properties of the bulk Bogoliubov-quasiparticle wave functions reflect themselves in different types of zero-energy vortex-bound states. In particular, in the case of NCSs with tetragonal point-group symmetry, we find that the stability of these Majorana zero modes is guaranteed by a combination of reflection, time-reversal, and particle-hole symmetries. Finally, by using K-theory arguments and a dimensional reduction procedure from higher-dimensional topological insulators and superconductors, we derive a classification of topologically stable Fermi surfaces in semimetals and nodal lines in superconductors.
To friends and family.
Acknowledgments

First of all, I would like to thank my advisor Shinsei Ryu for his guidance and education during the past 4 years. He has always been patient, encouraging, inspiring, and willing to sharing his valuable knowledge and insight with me. I learned a tremendous amount of physics from talking, discussing, and working with him. This dissertation would not be possible without his guidance.

I would like to thank Lance Cooper for his support and advice throughout my life as a graduate student at UIUC. I also would like to thank him for being my committee member.

I would like to thank my committee members: Taylor Hughes and Nadya Mason for being my thesis defense committee and their support on this thesis.

I have greatly benefited from my collaboration and numerous interactions with Andreas Schnyder, Shunji Matsura, and Christopher Mudry. I would like to thank them for their deep knowledge, sharp critical minds and friendly mentorships, which are invaluable for me.

I would also like to thank my UIUC friends: Mayukh Khan, Rodrigo Soto Garrido, Krishna Kumar, Grigoriy Polshyn, Olabode Sule, Xiao Chen, Xueda Wen, Chang-Tse Hsieh, AtMa Chan, Ching-Kai Chiu, Jeffrey Teo, Gil Young Cho, Hsiang-Hsuan Hung, Mao-Chuang Yeh, Xiongjie Yu, Victor Chua, Kridsanaphong Limtragool, Apoorv Tiwari, Vasilios Passias and many others in UIUC for many enjoyable times we shared.

Finally, I would like to express my sincere gratitude to my family: my parents, Jee-Sun Chang, Show-Zen Ro, and my wife, Yu-Ying Lee for their love and support. I would not have survived without them.
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6.2 (a) Hoppings of fermions between three consecutive sites \( r - 1, r, \) and \( r + 1 \) along a one-dimensional ring with four orbitals per site. A repeat unit cell is labeled by the integer \( r = 1, \ldots, N \) and is pictured by a rounded rectangular frame. A unit cell contains four orbitals that are pictured by black or white discs or squares, respectively. The hopping amplitude \( t + \delta t \in \mathbb{R} \) is pictured by a full connecting line. The hopping amplitude \( t - \delta t \in \mathbb{R} \) is pictured by a dashed connecting line. Hopping is only possible between orbitals of the same shape but distinct colors belonging to nearest-neighbor repeat unit cell. The figure is invariant under (i) the composition of the interchange of the full and dashed lines with the interchange of the black and white filling colors with a reflection about the horizontal dash-one-dot (red) line \( RH \) and (ii) the composition of the interchange of the circular and square shapes with a reflection about the vertical dash-two-dots (blue) line \( RVO \) if \( N \) is odd or the vertical dash-three-dots (green) line \( RVE \) if \( N \) is even. (b) Periodic boundary conditions are imposed (ring geometry) on the repeat unit cells represented by filled circles in the left panel, whereas open boundary conditions are imposed (open line geometry) on the repeat unit cells in the right panel. There are two physical boundaries on either sides of the cut represented by the dashed line and is odd or the vertical dash-three-dots (green) line \( RVE \) if \( N \) is even. (b) Periodic boundary conditions are imposed (ring geometry) on the repeat unit cells represented by filled circles in the left panel, whereas open boundary conditions are imposed (open line geometry) on the repeat unit cells in the right panel. The partitions \( A \) and \( B \) are made of the unit cells above and below the dashed line, respectively. There are two identical entangling boundaries an integer distance \( N/2 \) apart in the left panel. There are two identical physical boundaries a distance \( N \) apart in the right panel, each of which is an integer distance \( N/2 \) apart from a single entangling boundary.  

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6.4 The one-dimensional lattice model is defined by Fig. 6.2(a) with \( N := N_{\text{tot}}/N_{\text{orb}} = 48/4 = 12 \) repeat unit cells with either a torus or a cylindrical geometry. The partition is done by defining \( A \) and \( B \) to be the set of all the orbitals localized to the left (right) of the dash-three-dots (green) line \( RVE \) in Fig. 6.2(a). The equal-time-correlation matrix \( C \) is defined in Eq. (6.6). It is a \( 48 \times 48 \) Hermitian matrix with a \( 24 \times 24 \) Hermitian block defining the matrix \( C_A \), see Eq. (6.10c). The symmetry operation is the parity transformation (reflection) \( \mathcal{P} \) about the dash-three-dots (green) line \( RVE \) in Fig. 6.2(a). It interchanges \( A \) and \( B \) while leaving the entangling boundary \( RVE \) unchanged. Hence, \( \mathcal{P} \) can be represented by the \( 48 \times 48 \) matrix \( \mathcal{P} \) with the off-diagonal block structure displayed in Eq. (6.40b). The equal-time-correlation matrix \( C \) is defined in Eq. (6.6). It is a \( 24 \times 24 \) Hermitian matrix with a \( 24 \times 24 \) Hermitian block defining the matrix \( C_A \), see Eq. (6.10c). The symmetry operation is the parity transformation (reflection) \( \mathcal{P} \) about the dash-three-dots (green) line \( RVE \) in Fig. 6.2(a). It interchanges \( A \) and \( B \) while leaving the entangling boundary \( RVE \) unchanged. Hence, \( \mathcal{P} \) can be represented by the \( 48 \times 48 \) matrix \( \mathcal{P} \) with the off-diagonal block structure displayed in Eq. (6.40b). The equal-time-correlation matrix \( C \) is defined in Eq. (6.6). It is a \( 24 \times 24 \) Hermitian matrix with a \( 24 \times 24 \) Hermitian block defining the matrix \( C_A \), see Eq. (6.10c). The symmetry operation is the parity transformation (reflection) \( \mathcal{P} \) about the dash-three-dots (green) line \( RVE \) in Fig. 6.2(a). It interchanges \( A \) and \( B \) while leaving the entangling boundary \( RVE \) unchanged. Hence, \( \mathcal{P} \) can be represented by the \( 48 \times 48 \) matrix \( \mathcal{P} \) with the off-diagonal block structure displayed in Eq. (6.40b). The equal-time-correlation matrix \( C \) is defined in Eq. (6.6). It is a \( 24 \times 24 \) Hermitian matrix with a \( 24 \times 24 \) Hermitian block defining the matrix \( C_A \), see Eq. (6.10c). The symmetry operation is the parity transformation (reflection) \( \mathcal{P} \) about the dash-three-dots (green) line \( RVE \) in Fig. 6.2(a). It interchanges \( A \) and \( B \) while leaving the entangling boundary \( RVE \) unchanged.
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6.6 A cylinder of length $L$ along the $i + 1$ modulo 2 direction, while the coordinate $i = 1, 2$ has been compactified. We define two reflection planes. The first is defined by the blue frame that includes the cylinder axis. The second is defined by the red frame normal to the cylinder axis and intersecting the cylinder axis at its mid-point. The circles centered at the point L and R on the cylinder axis are the two disconnected boundaries of the cylinder. The reflection about the plane framed in blue leaves each circle invariant as a set. The reflection about the plane framed in red exchanges the circles centered on the cylinder axis at L and R. This plane framed in red defines the entangling boundary in a cylindrical geometry as defined by the partition (6.131).

6.7 Spectra $\sigma(\mathcal{H}_{k_1, \mu \nu}; \nu)$, $\sigma(Q_{k_1, \mu \nu}; A_{i+1})$, and $\sigma(\ln(Q_{k_1, \mu \nu}; A_{i+1} - 1))$ (with $i + 1$ defined modulo 2) for the single-particle Hamiltonian $\mathcal{H}_{k_1, \mu \nu}$ defined by the matrix elements (6.162) and the corresponding upper-left block $Q_{k_1, \mu \nu}; A_{i+1}$ from the equal-time one-point correlation matrix with $\nu = 2, 3$ taken from the fifth line from Table 6.4 (a) Spectrum $\sigma(\mathcal{H}_{k_1, \mu \nu}; \nu)$ for the linear sizes $M_1 = 128$ and $M_2 = 64$. (b) Scaling of the direct gap between the conduction bands at the momentum $k_1 = \pi/2$ and the mid-gap branch with positive energy eigenvalue at the momentum $k_1 = \pi/2$ as a function of increasing $M_2 = 16, 32, 64, 80, 96$ holding $M_1 = 128$ fixed. (c) Spectrum $Q_{k_1, \mu \nu}; A_{i+1}$ for the linear sizes $M_1 = 128$ and $M_2 = 64$. (d) Spectrum $\sigma(\ln(Q_{k_1, \mu \nu}; A_{i+1} - 1))$ for the linear sizes $M_1 = 128$ and $M_2 = 64$. (e) Spectrum $Q_{k_2, \mu \nu}; A_{i+1}$ for the linear sizes $M_1 = 64$ and $M_2 = 128$. (f) Spectrum $\sigma(\ln(Q_{k_2, \mu \nu}; A_{i+1} - 1))$ for the linear sizes $M_1 = 64$ and $M_2 = 128$. The coloring follows from the existence of the operator (6.164) that commutes with $Q_{k_2, \mu \nu}; A_{i+1}$. The coloring demonstrates the existence of a spectral flow that connects the valence to the mid-gap branches in the thermodynamic limit $M_1, M_2 \to \infty$.

6.8 The entanglement spectrum $\sigma(\hat{Q}_{k_1, \mu \nu})$ with $\hat{Q}_{k_1, \mu \nu}$ defined by Eqs. (6.180) and (6.181) for the spin quantum Hall effect. There are two branches of eigenstates with opposite chiralities (these chiralities are denoted by the colors blue and red) that cross at vanishing energy and momentum.

6.9 (a) The simplest tight-binding model for graphene with a Kekule distortion is defined by allowing spinless electrons to hop between any two nearest-neighbor sites of the honeycomb lattice with the real-valued modulated amplitudes $t_1$ and $t_2$ if a nearest-neighbor bond is colored in red or blue, respectively. The repeat unit cell of the strong and weak bonds associated to the Kekule distortion can be chosen to be made of the following three hexagons below the dashed line. The first hexagon is colored in blue and has six vertices numbered clockwise from 1 to 6. The second hexagon shares the bond $\langle 12 \rangle$ with the first one. The third hexagon shares the bond $\langle 23 \rangle$ to the first one. This unit cell comprised of these three hexagons is three time as large as the repeat unit cell of the honeycomb lattice with all nearest-neighbor bonds colored in black (the limiting case when $t_1 = t_2$). This enlarged repeat unit cell has 6 inequivalent sites. The spanning vectors of the honeycomb lattice with the Kekule coloring of nearest-neighbor bonds are $\alpha_1$ and $\alpha_2$. (b) The large hexagon colored in black defines the first Brillouin zone of the triangular lattice. The small hexagon colored in blue defines the first Brillouin zone of the honeycomb lattice with the Kekule coloring of nearest-neighbor bonds. The ratio of the area of the black hexagon to the area of the blue hexagon is three to one. If the honeycomb lattice is cut along the horizontal dashed line, an armchair edge is obtained. The point denoted by $\bullet$ at the mid-point where the dashed line intersects the nearest-neighbor bond coming out of vertex 1 below the dashed line defines the inversion center. The points $\Gamma, M_1, M_2$ and $M_3$ from the first Brillouin zone of the honeycomb lattice with the Kekule coloring of nearest-neighbor bonds are invariant (fixed) under this inversion.
6.10 Energy spectrum of Hamiltonian \((6.197)\) with armchair edges for (a) \((t_1, t_2) = (1/3, 4/3)\) and (b) \((t_1, t_2) = (5/3, 2/3)\). Entanglement spectrum with armchair entangling edges for (c) \((t_1, t_2) = (1/3, 4/3)\) and (d) \((t_1, t_2) = (5/3, 2/3)\). The dimensions of the lattice are given by \((N_1, N_2) = (128, 32)\), where \(N_i\) is the number of the repeat unit cell from Fig. 6.9(a) along the direction of the spanning vector \(a_i\) \((i = 1, 2)\) and in units for which the spanning vectors \(a_1\) and \(a_2\) are of unit length.

6.11 Energy spectra are presented in the left column, entanglement spectra are presented in the right column. In both cases, the geometry is that of a slab with armchair edges as in Fig. 6.9(a) for \((t_1, t_2) = (5/3, 2/3)\) and \((N_1, N_2) = (128, 32)\). The spectra (a) and (d) are obtained by choosing the time-reversal-breaking perturbation \((6.209)\) in Hamiltonian \((6.208)\). The spectra (b) and (e) are obtained by choosing the chiral-symmetry-breaking perturbation \((6.210)\) with \((6.212)\) in Hamiltonian \((6.208)\). The spectra (c) and (f) are obtained by choosing the inversion-symmetry-breaking perturbation \((6.213)\) to Hamiltonian \((6.208)\).

6.12 (a) The nearest-neighbor bonds of the honeycomb lattice are colored in red, blue, and green as depicted. The colors red, blue, and green correspond to the values \(t_1\), \(t_2\), and \(t_3\) taken by the nearest-neighbor hopping amplitudes for spinless fermions hopping on the honeycomb lattice with Hamiltonian \((6.226)\), respectively. The repeat unit cell with its spanning vectors \(a_1\) and \(a_2\) was defined in Fig. 6.9(a). An armchair entangling edge is obtained by opening the honeycomb lattice through the dashed line. (b) The cylindrical geometry with the two armchair edges differing by their colors is pictured. The colors red, blue, and green correspond to the values \(t_1\), \(t_2\), and \(t_3\) taken by the nearest-neighbor hopping amplitudes \(t_1\), \(t_2\), \(t_3\), and \(t_2\). The top armchair edge denoted by a red ellipse has fermions hopping along it with the consecutive hopping amplitudes \(t_1\), \(t_2\), \(t_3\), and \(t_2\). The bottom armchair edge denoted by the blue ellipse has fermions hopping along it with the consecutive hopping amplitudes \(t_1\), \(t_3\), \(t_2\), and \(t_3\). [Note that these are not the armchair boundaries shown in panel (a).]

6.13 (a) Energy spectrum with two armchair edges in the cylindrical geometry of Fig. 6.12(b). (b) Entanglement spectrum with two entangling armchair boundaries in a toroidal geometry. The energy scales are \(\Delta_0 = 1\) and \(t = -1\). The axial phase is \(\alpha \cong 6.927\). The lattice size is \((N_1, N_2) = (128, 32)\). The number of unit cells along \(a_1\) is \(N_i\) for \(i = 1, 2\).

6.14 The nearest-neighbor bonds of the honeycomb lattice are colored in red and blue as depicted. The colors red and blue correspond to the values \(t_1\) and \(t_2\) taken by the nearest-neighbor hopping amplitudes for spinless fermions hopping on the honeycomb lattice with Hamiltonian \((6.230)\), respectively. A Kekule distortion follows from choosing \(t_1 \neq t_2\). A physical zigzag edge is constructed from cutting through the dashed line. The dashed line also defines a zigzag entangling edge. The symbol \(\bullet\) denotes an inversion center. One repeat unit cell contains three hexagons defined as follows. The first hexagon from the repeat unit cell has two sites numbered 1 and 2, whereby site 1 is connected by a blue bond to site 2. The second hexagon from the repeat unit cell has three sites numbered 2, 3, and 4, whereby site 2 is connected by a blue bond to site 3, while site 3 is connected by a red bond to site 4. The third hexagon from the repeat unit cell has all six edges colored in blue with the vertices numbered 4, 5, and 6. The spanning vectors corresponding to this unit cell are \(a_1\) and \(a_2\). The image of the repeat unit cell under inversion about the point \(\bullet\) is has its three hexagons labeled with the numbers 1 to 6 written upside down.

6.15 Energy spectra of \(\mathcal{H}_{\text{zig}} k_{\|}\) in Eq. \((6.235)\) with zigzag edges in a cylinder geometry for (a) \((t_1, t_2) = (1/3, 4/3)\) and (b) \((t_1, t_2) = (5/3, 2/3)\). Entanglement spectra of \(\mathcal{H}_{\text{zig}} k_{\|}\) in Eq. \((6.235)\) with zigzag entangling edges in a torus geometry for (c) \((t_1, t_2) = (1/3, 4/3)\) and (d) \((t_1, t_2) = (5/3, 2/3)\). The dimensions of the lattice are given by \((N_1, N_2) = (128, 32)\), where \(N_i\) is the number of the repeat unit cell from Fig. 6.14 along the direction of the spanning vector \(a_i\) \((i = 1, 2)\) and in units for which the spanning vectors \(a_1\) and \(a_2\) are of unit length.
Energy spectra of $H_k$ in Eq. (6.235) with zigzag edges in a cylindrical geometry are presented in the left column. Entanglement spectra of $H_k$ in Eq. (6.235) with zigzag entangling edges in a torus geometry are presented in the right column. In both cases, we set $(t_1, t_2) = (5/3, 2/3)$ and $(N_1, N_2) = (128, 32)$. The spectra (a) and (d) are obtained by choosing the inversion-breaking perturbation (6.236) in Hamiltonian (6.235). There are mid-gap flat bands that are two-fold degenerate. The spectra (b) and (e) are obtained by choosing the chiral-symmetry-breaking perturbation (6.237) in Hamiltonian (6.235). The flat bands remain two-fold degenerate but are shifted away from zero energy in panel (b). The spectra (c) and (f) are obtained by choosing both the inversion-symmetry-breaking and chiral-symmetry-breaking perturbation (6.238) to Hamiltonian (6.235). The two-fold degeneracy of the flat bands is lifted and all flat bands are shifted away from the eigenvalue zero in panels (c) and (f).

B.1 (Color online). Energy spectrum as a function of $k_z$ of a $C_4v$ NCS with $(a_1, a_2) = (1.0, 2.0)$, $\mu = -2.5$, and $\Delta_s = 0.5$. (a) Without vortices and PBC along the $x$ axis but OBC in the other two directions. (b) With a pair of vortex-antivortex lines oriented along the $z$ axis and PBCs in all three directions.
<table>
<thead>
<tr>
<th>Abbreviation</th>
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<tr>
<td>AZ</td>
<td>Altland-Zirnbauer</td>
</tr>
<tr>
<td>Bz</td>
<td>The first Brillouin Zone</td>
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<tr>
<td>h.c.</td>
<td>Hermitian Conjugate</td>
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<tr>
<td>TRS</td>
<td>Time-Reversal Symmetry</td>
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<tr>
<td>PHS</td>
<td>Particle-Hole Symmetry</td>
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<tr>
<td>IS</td>
<td>Inversion Symmetry</td>
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<tr>
<td>TI</td>
<td>Topological Insulator</td>
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<tr>
<td>TSC</td>
<td>Topological superconductor</td>
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<tr>
<td>NCS</td>
<td>Noncentrosymmetric superconductor</td>
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<td>SOC</td>
<td>Spin-orbit coupling</td>
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List of Symbols

$\mathcal{K}$ Conjugate operator
$I$ Identity matrix
$\sigma_i$ Pauli matrices
$T$ Time-reversal symmetry operator
$P$ Particle-hole symmetry operator
$S$ Chiral symmetry operator
$\nu_1$ One-dimensional winding number
$\nu_3$ Three-dimensional winding number
$d_{\text{BZ}}$ Total dimension of BZ
$d_k$ (codimension of a Fermi surface)−1
$d_r$ (codimension of a real space defect)−1
Chapter 1

Introduction

1.1 Background and motivation

One great triumph in contemporary condensed matter physics is the discovery of the topological phases of matter. Topological materials, such as the integer quantum Hall state and the topological insulators (superconductors), are characterized by the topology of their ground state, which gives rise to protected gapless boundary states and quantized electrical and gravitational responses [1–5]. The properties of topological materials are invariant under small perturbations and cannot be continuously connected to the trivial phase without closing the energy gap. Moreover, topological materials cannot be characterized by a broken symmetry because of their property of quantum entanglement. Many topological phenomena, such as magneto-electric effects [7], localized Majorana fermions [8], and spin transport are predicted to exist in these systems. These phenomena can lead to interesting technical applications, such as spintronic devices and quantum computation.

Besides fully gapped topological materials, robust topological properties can also exist for the systems that have stable Fermi points or nodal lines in the energy spectrum. These gapless phases can also host protected zero-energy boundary states that can be either dispersive (e.g., surface Dirac/Majorana cones) or dispersionless (e.g., surface flat bands and Fermi-arc states). Examples of these gapless systems are Dirac points in graphene [9][14], Fermi arcs in unconventional superconductors [15][20], the A phase of superfluid $^3$He [21][22], Weyl semimetals [23][36], and nodal noncentrosymmetric superconductors (NCSs) [37][48].

Gapless topological phases with Fermi points such as Weyl semimetals have been extensively studied. Many proposed materials of Weyl semimetals including $\text{R}_2\text{Ir}_2\text{O}_7$, $\text{HgCr}_2\text{Se}_4$, $\text{TaAs}$, $\text{SrSi}_2$, $\text{NbAs}$ show multi Fermi points in the bulk spectrum. The protected Fermi-arc states have also been observed experimentally by ARPES measurements [34][35]. Many interesting topological transport properties also exist in Weyl semimetals, such as the magnetic-field-driven current [49][52] and the negative magnetoresistivity [56]. Unlike Weyl semimetals, many gapless topological phases such as semimetals with Fermi lines and nodal superconductors with nodal lines have not been well studied. Our main motivation is to go beyond gapless topological phases with Fermi points by focusing on the nodal superconductors with nodal lines in three dimensions. Moreover, we also want to give a general classification of these gapless phases.
in arbitrary dimensions under different discrete symmetries, e.g., time-reversal, particle-hole, and chiral symmetries. In this thesis, we specifically focus on three dimensional nodal NCSs. In the presence of broken inversion symmetry, strong spin-orbit coupling, and an admixture of spin-singlet and triplet pairing states, NCSs can exhibit topologically nontrivial characteristics. To reveal the topological properties of these nodal superconductors, we focus on studying the symmetry protected surface and vortex states in nodal NCSs.

1.2 Methods and Main results

To study the surface states of nodal NCSs, we use exact diagonalization of the Bogoliubov-de Gennes (BdG) Hamiltonians. We demonstrate the existence of surface flat bands originated from the nodal lines in the bulk. The presence of surface flat bands can lead to a zero-energy divergence in surface density of states. This divergence can be measured as a zero-bias peak in the surface tunneling conductance. In addition to the surface flat bands, we investigate zero-energy Majorana vortex-bound states in three dimensional fully gapped and nodal NCSs by combining analytical solutions of the Bogoliubov-de Gennes (BdG) equations in the continuum with exact diagonalization of the BdG Hamiltonian. Remarkably, we find that different crystal point-group symmetries lead to different types of zero-energy Majorana vortex-bound states. We show that in the case of the $C_4v$ ($D_4$) point group, the stability of these Majorana zero modes is guaranteed by a combination of reflection ($\pi$ rotation), time-reversal, and particle-hole symmetries. Furthermore, by considering continuous deformations of the quasiparticle spectrum in the presence of vortices, the vortex bound states of NCSs with $D_4$ point-group symmetry have dispersive vortex-bound states that can be adiabatically connected to time-reversal symmetric topological superconductors. On the other hand, NCSs with $C_4v$ point-group symmetry exhibit dispersionless vortex-bound states that can be connected to time-reversal symmetric Weyl superconductors.

Next, we derive a classification of topologically stable Fermi surfaces in semimetals and superconductors using K-theory arguments and a dimensional reduction procedure from higher-dimensional topological insulators and superconductors. The former method of classifying topological phases in these gapless systems is (1) to treat the gapless points as defects, (2) to adiabatically go around the defects (e.g., a loop circling around a line defect or a sphere encircling a point defect), and (3) to monitor the wave functions apart from the defects. The latter method is to interpret topological stable gapless points in $d$ dimensions as the surface states of $(d + 1)$-dimensional topological insulators. The classification table is given in Table 5.3.

Finally, we would like to add one chapter, describing the entanglement properties of crystalline topological insulators[53]. We will show that the entanglement spectrum is a very useful tool to diagnose the topological insulators protected by point-group symmetries. We first show that a Hermitian operator obeying supersymmetric quantum
mechanisms (SUSY QM) delivers the entanglement spectrum. We then show that such an entanglement spectrum that is compatible with a certain point-group symmetry obeys a certain local spectral symmetry. The latter result is applied to the stability analysis of four fermionic non-interacting Hamiltonians, the last of which describes graphene with a Kekule distortion. All examples have the remarkable property that their entanglement spectra inherit a local spectral symmetry from either an inversion or reflection symmetry that guarantees the stability of gapless boundary entangling states, even though all examples fail to support protected gapless boundary states at their physical boundaries.

1.3 Thesis overview

The rest of the thesis is organized as follows: An introduction to gapless topological semimetal and nodal superconductors is given in Chapters 2 and 3. As a warm up, we review models of Weyl semimetals and $^3$He A-phase with point nodes and their corresponding surface arc states in Chapter 2. A time-reversal-invariant nodal superconductor with spin $S_z$ conservation and nodal NCSs, which have surface flat bands, will be discussed in Chapter 3. In chapter 4, we investigate surface and vortex states in three-dimensional nodal NCSs. In chapter 5, a classification table of topological gapless phases is derived. In chapter 6, we investigate the symmetry-protected zero modes in the entanglement spectrum for topological insulators protected by spacial symmetries. In chapter 7, we conclude our main results and give future prospect of these interesting gapless topological states of matter.
Chapter 2

Protected surface arc states in Weyl semimetals and A-phase of superfluid $^3$He

2.1 Introduction

Many interesting gapless phases (e.g., semimetals and nodal superconductors) exhibit Fermi points in the bulk. One famous example is graphene, which the low energy excitation can be expressed by the two-dimensional Dirac Hamiltonian. The Dirac Hamiltonian has linear energy dispersion at Dirac (Fermi) points, which are denoted the band-touching points in the BZ. In three dimensions, Weyl semimetals and A-phase of superfluid $^3$He also have Fermi points in the bulk. One nature question arises, "Why these Fermi points are robust?" The stability of these Fermi points can be understood from a topological point of view, i.e., Fermi points can be seen as topological defects in momentum space. It turns out one can define topological charges (topological invariants) associated with Fermi points. The Fermi points in Weyl semimetals are the sources and drains of Berry flux\(^1\) [see Fig. 2.1(a)]. The topological invariants are determined by the topology the wave function on a two-dimensional sphere encircling the Fermi point [see Fig. 2.1(b)]. This two-dimensional topological invariant is the Berry curvature [see App. A.1.1]. Since the Fermi points are sources and drains of Berry flux, any surface encircling the Fermi point will have non-vanishing Chern number. The topological charge of the Fermi point is given by the Chern number on a sphere encircling this Fermi point. Due to the non-vanishing Chern number of each sphere encircling the Fermi point, zero-energy arc states appear on the surface. These surface arc states connect projections of Fermi points with opposite topological charges on the surface BZ [see Fig. 2.1(c)]. We consider a continuous deformation of the sphere encircling the Fermi point from the light green sphere to the light orange surface and to the light purple sheet in Fig. 2.1(b). This deformation will not change the value of the Chern number as long as the surface encircles the Fermi point. These surfaces can be seen as two-dimensional Chern insulators with non-trivial topological characteristics. These Chern insulators have chiral edge modes once the boundary is introduced. The appearance of zero-energy arc states can be understood from the zero-energy states from each chiral mode of each Chern insulator. The non-vanishing topological charges of the Fermi points give rise to the existence of zero-energy arc states — a generalized bulk-boundary correspondence. We will examine this generalized bulk-boundary correspondence by two examples: Weyl semimetals and A-phase of superfluid $^3$He in the following

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\(^1\)The definition of Berry flux is in App. A.1.1
Figure 2.1: (a) The blue arrows are the direction of Berry flux going from the top Fermi point to the bottom Fermi point, where the Fermi points are indicating by red points. (b) Light purple sheet, light orange sheet, and light green sphere encircle the upper Fermi point. (c) The brown plane represent the two-dimensional surface BZ parametrized by the two surface momenta $k_1$ and $k_2$. $\pm 1$ indicates the topological charge of each Fermi point. The green line shows regions in the surface BZ where there appear zero-energy arc states.

2.2 Weyl semimetals

Weyl semimetals can be seen as a three-dimensional analogs of graphene. Potentially, Weyl semimetals can be realized in transition metal oxides with strong spin-orbit coupling\cite{25, 27, 28}, heterostructures\cite{26}, or stoichiometric materials\cite{32, 33}. The Fermi points in Weyl semimetals can be described by the $2 \times 2$ Hamiltonian of chiral Weyl fermions, $\mathcal{H} = k_x \sigma_x + k_y \sigma_y + k_z \sigma_z$. Without breaking time-reversal symmetry (TRS) or inversion symmetry (IS), Weyl points are doubly degenerate due to the Kramers theorem. In order to make Weyl semimetals, we need to break either TRS or IS. Without loss of generality, we consider a two-band model breaks TRS introduced in Ref.\cite{54}

$$\mathcal{H}(k) = [2t(\cos k_z - \cos k_0) + m(2 - \cos k_y - \cos k_x)] \sigma_z + 2t \sin k_y \sigma_y + 2t \sin k_x \sigma_x. \quad (2.1)$$

We set $t = 1$ and $m = -2$ such that there are two Fermi points locating $(0, 0, \pm k_0)$ [see Fig. 2.2(a), two Fermi points locate at $(0, 0, \pm \pi/2)$]. The Chern number is well defined for any Hamiltonian on a two-dimensional surface embedded in three-dimensional BZ, as long as the two-dimensional surface does not across the Fermi points. Let us fix $k_z$ for defining a two-dimensional Hamiltonian $\mathcal{H}_{k_z}(k_x, k_y)$ and compute the corresponding Chern number. It turns out, for $k_z \in (-k_0, k_0)$, the Chern number $C = 1$ and $C = 0$ otherwise. The non-vanishing Chern number ($C = 1$) indicates there must be a chiral edge state for each two-dimensional Hamiltonian $\mathcal{H}_{k_z}(k_x, k_y)$ at fixed $k_z \in (-k_0, k_0)$. The consequence of these chiral edge states leads to a surface arc state connecting the Fermi points in the surface BZ [see Fig. 2.2(b)].
Figure 2.2: (a) and (c): Energy spectrum as a function of $k_z$ under period boundary conditions along $x$, $y$, and $z$ directions. (b) and (d): Energy spectrum as a function of $k_z$ under period boundary conditions along $y$ and $z$ directions, and an open boundary conduction along $x$ direction. Upper panels (a) and (b) correspond to the model of Weyl semimetals. Lower panels (c) and (d) correspond to the model of $^3$He A-phase.

2.3 Superfluid $^3$He A-phase

Let us consider superfluid $^3$He A-phase as another example. Unlike $^3$He B-phase with isotropic order parameter, which is a fully gapped system, $^3$He A-phase exhibits nodal points in the quasiparticle energy spectrum. In $^3$He, the order parameter is a triplet pairing, $\Psi = (d_x |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + id_y (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) + dz (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle))(k_x + ik_y)$, with $d = (d_x, d_y, d_z)$ denoting the d-vector. In A-phase of $^3$He, the d-vector is $d = (\Delta_0, \Delta_0, 0)$, with spin-up and spin-down pairs having the same amplitude $\Delta_\uparrow = \Delta_\downarrow = \Delta_0$. Since there is no pairing between spin-up and spin-down, we can simplify the model by considering only one spin component. The BdG Hamiltonian $H = \frac{1}{2} \sum_k \phi_k^\dagger \mathcal{H}(k) \phi_k$ with $\phi_k = (c_k, c_k^\dagger)^T$ is

$$\mathcal{H}(k) = \begin{pmatrix} h(k) & \Delta(k) \\ \Delta^\dagger(k) & -h^T(-k) \end{pmatrix}, \quad \tag{2.2}$$

where

$$h(k) = 2t (\cos k_x + \cos k_y + \cos k_z) - \mu, \quad \Delta(k) = \Delta_0 (\sin k_x - i \sin k_y), \quad \tag{2.3}$$
with $\Delta_0$ being the amplitude of the triplet pairing. Here, we consider a cubic lattice model with the hopping amplitude in the normal state being $t$ and the chemical potential being $\mu$. The energy spectrum of the BdG Hamiltonian is

$$\lambda_k^\pm = \pm \sqrt{(2t(cos k_x + cos k_y + cos k_z) - \mu)^2 + \Delta_0^2(sin^2 k_x + sin^2 k_y).} \quad (2.4)$$

For $\frac{\mu}{2t} - 2 \in (-1, 1)$, there are two nodal points at $(0, 0, \cos^{-1}(\frac{\mu}{2t} - 2))$ in BZ [see Fig. 2.2(c)]. Similar to the Weyl semimetal described in Eq. (2.1), the Chern number of any embedded Hamiltonian $H_{k_z}(k_x, k_y)$ at fixed $k_z \in (-\cos^{-1}(\frac{\mu}{2t} - 2), \cos^{-1}(\frac{\mu}{2t} - 2))$ is $C = 1$, i.e., this embedded Hamiltonian describes a two-dimensional topological superconductor. For each two-dimensional topological superconductor, there must be a chiral Majorana edge state. Hence there is a surface arc state connecting projections of nodal points on the surface BZ [see Fig. 2.2(d)].

### 2.3.1 Vortex flat bands in $^3$He A-phase

As pointing out by Volovik[21], a flat band can emerge in the core of a vortex in the $^3$He A-phase. This flat-band vortex state is determined by projections of the nodal points in the bulk to the vortex axis — a bulk-vortex correspondence. We investigate the appearance of flat-band vortex states in the $^3$He A-phase by introducing a pair of vortex and anti-vortex in Eq. (2.2).

Vortex lines can be introduced by adding phase angle $\phi(r_\perp)$ on the pairing term, $\Delta_0 \rightarrow \Delta(r_\perp) = \Delta_0 e^{i\phi(r_\perp)}$. We assume the system is translational invariance along the vortex lines which is normal to $r_\perp$, and $k_\parallel$ is the momentum along the vortex lines. The single particle BdG Hamiltonian can be expressed as

$$\mathcal{H}(r_\perp, r'_\perp, k_\parallel, \phi(r_\perp)) = \begin{pmatrix} h(r_\perp, r'_\perp, k_\parallel) & \Delta_0(r_\perp, r'_\perp, k_\parallel) e^{i\phi(r_\perp)} \\ \Delta_0^*(r_\perp, r'_\perp, k_\parallel) e^{-i\phi(r_\perp)} & -h^T(r_\perp, r'_\perp, k_\parallel) \end{pmatrix}. \quad (2.5)$$

We consider a lattice model in the presence of a vortex-antivortex pair under periodic boundary conditions along $x, y, z$ directions. Assuming the vortex-antivortex pair is along $z$ direction, this phase angle $\phi(r_\perp)$ can be parametrized as

$$\phi(r_\perp) = \tan^{-1} \frac{2aby}{x^2 + (by)^2 - a^2}, \quad (2.6)$$

where the vortex and the antivortex locate at $(a, 0)$ and $(-a, 0)$ on the $x - y$ plane, and $b$ is the parameter that characterizes the shape of this vortex-antivortex pair. Notice the vorticity for the vortex is $+1$ and for the anti-vortex is $-1$.\[7\]
In the numerical setup, we consider $N \times N$ lattice sites in $x - y$ plane. The normal states Hamiltonian and the pairing term in momentum space in the absence of the vortex-antivortex pair are expressed as, $h(k) = h_1 e^{ikx} + h_1^* e^{-ikx} + h_2 e^{iky} + h_2^* e^{-iky} + h_3(k_z)$, $\Delta(k) = \Delta_1 e^{ikx} + \Delta_1^* e^{-ikx} + \Delta_2 e^{iky} + \Delta_2^* e^{-iky} + \Delta_3(k_z)$, respectively. Then, the BdG Hamiltonian in $(r_x, k_z)$ spaces in the presence of the vortices is

$$\mathcal{H}(r_x, r_y, k_z) = (I_{N \times N} \otimes I_{N \times N}) \otimes \begin{pmatrix} h_3(k_z) & 0 \\ 0 & -h_3^T(k_z) \end{pmatrix} + \{\delta_{(i-1)N+j, (i-1)N+j} e^{i\phi(i,j)} \otimes \begin{pmatrix} 0 & \Delta_3(k_z) \\ 0 & 0 \end{pmatrix} + h.c.\}$$

$$+ \{\mathbb{B} \otimes I_{N \times N} \otimes \begin{pmatrix} h_1 & 0 \\ 0 & -h_1^T \end{pmatrix} + \mathbb{B} \otimes I_{N \times N} \otimes \begin{pmatrix} h_2 & 0 \\ 0 & -h_2^T \end{pmatrix}$$

$$+ \delta_{(i-1)N+j, (i-1)N+1} e^{i\phi(i,j)} \otimes \begin{pmatrix} 0 & \Delta_1 \\ 0 & 0 \end{pmatrix} + e^{-i\phi(i,j)} \otimes \begin{pmatrix} 0 & 0 \\ 0 & \Delta_1^T \end{pmatrix}$$

$$+ \delta_{(i-1)N+j, \text{Mod}(i, N)+j} e^{i\phi(i,j)} \otimes \begin{pmatrix} 0 & \Delta_2 \\ 0 & 0 \end{pmatrix} + e^{-i\phi(i,j)} \otimes \begin{pmatrix} 0 & 0 \\ 0 & \Delta_2^T \end{pmatrix} + h.c.\}, \quad (2.7)$$

where

$$\mathbb{B} = \begin{pmatrix} 0 & 1 & \cdots & 0 \\ \vdots & 0 & 1 & 0 \\ & & \ddots & \vdots \\ & & & 0 \\ 1 & \cdots & & 0 \end{pmatrix}, \quad (2.8)$$

and $i, j$ are the site labels corresponding to the space coordinate, $x = j - \frac{N+1}{2}$ and $y = \frac{N+1}{2} - i$.

The vortex-antivortex pair is introduced along $z$ direction with the vortex and anti-vortex locating at $(a, 0)$ and $(-a, 0)$ on $x - y$ plane, respectively. We consider $N = 50$ sites and set $a = 8$, $b = 2$. The flat-band vortex states emerge in the presence of the vortex-antivortex pair as shown in Fig. 2.3(a). Notice that in the absence of vortices, the embedded Hamiltonian $\mathcal{H}_{k_z}(k_x, k_y)$ is a two-dimensional topological superconductors for fixed $k_z \in (-\cos^{-1}(\frac{\mu}{2T} - 2), \cos^{-1}(\frac{\mu}{2T} - 2))$. For each embedded Hamiltonian $\mathcal{H}_{k_z}(k_x, k_y)$, zero-energy vortex states can emerge in the presence of vortices. Hence flat-band vortex states in $^3$He A-phase arise from connecting all the zero-energy vortex states in the embedded Hamiltonian $\mathcal{H}_{k_z}(k_x, k_y)$ for fixed $k_z \in (-\cos^{-1}(\frac{\mu}{2T} - 2), \cos^{-1}(\frac{\mu}{2T} - 2))$. The stability
of the flat-band vortex states is characterized by the $\mathbb{Z}_2$ topological invariant \cite{21, 55}

$$\nu = CV \mod 2,$$

(2.9)

where $C$ is the Chern number of the embedded Hamiltonian $H_{k_z}(k_x, k_y)$ and $V$ is the vorticity associated with the vortex. In our case, the Chern number is always one, $C = 1$. The $\mathbb{Z}_2$ property of the flat-band vortex states in the core of the vortex-antivortex pair appears when we change the parity of vorticities of the vortex and the antivortex. For $V = 2$, there is no flat-band vortex state as shown in Fig. 2.3(b). For $V = 3$, the flat-band vortex states appear again as shown in Fig. 2.3(c).

### 2.4 Summary

In summary, we demonstrate the existence of surface arc states for topological gapless phases with Fermi points. The origin of these arc states arises from the topological characteristics of Fermi points, which can be seen as sources or drains of Berry flux in the momentum space. This phenomenon is a generalized bulk-boundary correspondence in gapless phases with Fermi points. In addition, we demonstrate a bulk-vortex correspondence in $^3$He A-phase. The flat-band vortex states connect projections of the Fermi points in the bulk to the vortex axis.
Chapter 3

Protected surface flat bands in nodal topological superconductors with nodal lines

3.1 Introduction

Many nodal superconductors exhibit line nodes in the bulk, which can be experimentally measured from thermal transport [56], penetration depth [57], and NMR spin relaxation rate [58]. To understand the stability of nodal lines in three-dimensional nodal superconductors, we apply a general derivation of topological invariants that characterize the stability of nodal lines in these systems [see App. A.1.2 and Refs. [6, 7, 40, 59–63]]. For nodal lines in three dimensions, the topological characteristics of the nodal line are determined by the topology of the wavefunction along a closed loop that encircles the nodal line [see Fig. 3.1(b)]. This topological invariant is characterized by the one-dimensional winding number \( \nu_1 \) [see App. A.1.2]. Since the nodal lines can be seen as the flux tubes in the momentum space [see Fig. 3.1(a)], where the flux is the Berry flux \( \mathbf{B} \), the winding number of the loop will be non-vanishing for the loop that encircles the nodal line. Due to non-vanishing wind numbers of each nodal ring, zero-energy states appear within regions of the surface BZ that are bounded by the projected bulk nodal rings. The appearance of the surface flat-bands can be understood by considering a continuous deformation of the closed grey loop to the black dashed loop in Fig. 3.1(b). The deformation of the loop does not change the value of winding number computed from the loop, as long as the loop encircles the nodal ring. We can treat this loop as a one-dimensional gapped Hamiltonian with non-trivial topological characteristics. Once a boundary is introduced in the system, the must be zero-energy states at the ends of each one-dimensional gapped Hamiltonian. The zero-energy states occur in two-dimensional regions in the surface BZ that are bounded by the projection of the bulk nodal rings [Fig. 3.1(c)]. These surface flat-bands are originated from the non-trivial topological properties of the bulk nodal rings. This phenomenon is a generalized bulk-boundary correspondence. In the following sections, we examine topologically stable nodal lines in three-dimensional time-reversal invariant superconductors with and without spin-\( S^z \) conservation. The robustness of the nodal lines and the associated topological surfaces states against disorder is discussed in Sec. 3.4.

\[ \nu = \frac{1}{2\pi} \oint_{L} dk_\mu \text{Tr}[A_\mu] = \frac{1}{2\pi} \int ds \cdot \mathbf{B}, \]

where \( L \) is a closed integral path encircling the nodal ring, \( A_\mu \) is the Berry connection and \( \mathbf{B} \) is the Berry flux. See the detail definitions in App. A.1.1.
Figure 3.1: (a) The blue arrows are the direction of Berry flux winding along the nodal rings (red circles). (b) Grey and black loops encircle the upper nodal ring (red circle). (c) The brown plane represent the two-dimensional surface BZ parametrized by the two surface momenta $k_{1\parallel}$ and $k_{2\parallel}$. ±1 corresponds to the topological charge of each nodal ring. The red and green areas indicate regions in the surface BZ where there appear zero-energy states.

3.2 Nodal topological superconductors with spin-$S^z$ conservation

As a first example, we study a three-dimensional time-reversal invariant superconductor with spin-$S^z$ conservation described by the BdG Hamiltonian $H = \frac{1}{2} \sum_k \psi_k^\dagger H_4(k) \psi_k$, with $\psi_k = (c_{k\uparrow}, c_{k\downarrow}, c_{-k\uparrow}^\dagger, c_{-k\downarrow}^\dagger)^T$. Rotational symmetry about the $z$-axis in spin space is implemented by $[H_4(k), J_z] = 0$, with $J_z = \text{diag}(\sigma_3, -\sigma_3^T)$. Hence, the $4 \times 4$ Hamiltonian $H$ can be brought into block diagonal form, $\tilde{H} = \frac{1}{2} \sum_k \tilde{\psi}_k^\dagger \tilde{H}_4(k) \tilde{\psi}_k$, where $\tilde{H}_4(k) = \text{diag}[H_2(k), -H_2(-k)]$ and $\tilde{\psi}_k = (c_{k\uparrow}, c_{-k\downarrow}^\dagger, c_{-k\uparrow}^\dagger, c_{k\downarrow})^T$. It follows that the topology of $H_4(k)$ is fully determined by the topology of $H_2(k)$.

For concreteness, we consider

$$
\tilde{H}_2(k) = \begin{pmatrix}
\varepsilon_k + \alpha l_z^k & \Delta_s + \Delta l_z^k \\
\Delta_s + \Delta l_z^k & -\varepsilon_k - \alpha l_z^k
\end{pmatrix}
$$

The normal part of this Hamiltonian, $\varepsilon_k + \alpha l_z^k = 2t (\cos k_x + \cos k_y + \cos k_z) - \mu + \alpha \sin k_z$, describes electrons hopping between nearest-neighbor sites of a cubic lattice with hopping amplitude $t$, chemical potential $\mu$, and spin-orbit coupling strength $\alpha$. The superconducting order parameter contains both even-parity spin-singlet and odd-parity spin-triplet components, denoted by $\Delta_s$ and $\Delta l_z^k = \Delta t \sin k_z$, respectively. Due to the presence of time-reversal symmetry the gap functions are purely real, and hence $\tilde{H}_2(k)$ anticommutes with $\sigma_2$, i.e., $\{\tilde{H}_2(k), \sigma_2\} = 0$. Therefore, $\tilde{H}_2(k)$ belongs to symmetry class AIII and we find that this system can exhibit stable nodal lines (see Table 5.3). Indeed, the energy spectrum of Eq. (3.1), $\lambda_k^\pm = \pm \sqrt{(\varepsilon_k + \alpha l_z^k)^2 + (\Delta_s + \Delta l_z^k)^2}$, shows a nodal ring, which is

\footnote{This model is equivalent to the polar state of $^3$He [64]. A two-layer version of this model might be realized in the pnictide superconductor SrPtAs [65,67].}
located within the \((k_x,k_y)\)-plane and centered around the \(k_z\) axis [Fig. 3.2(a)]. The nodal line is described by the manifold

\[
\{k \in \text{BZ}; \text{ with } k_z = 0 \text{ and } k_x = \pm \arccos \left[ \frac{\mu}{t} - 1 - \cos k_y \right] \}.
\]

(3.2)

The topological stability of this nodal ring is characterized by the winding number \(\nu_1\), Eq. (A.15). Evaluating \(\nu_1\) for Hamiltonian (3.1) gives

\[
\nu_1 = \frac{1}{2\pi \text{Im}} \int_{S^1} dk \text{Tr} \{ \partial_k \ln [\varepsilon_k - i\Delta_s + (\alpha - i\Delta_t) l_z^k] \},
\]

(3.3)

where \(S^1\) represents a circle in momentum space. We find that \(\nu = \pm 1\), whenever \(S^1\) interlinks with the nodal ring \(3.2\). It is shown in Sec. 5.2.5 topologically nontrivial nodal lines of codimension \(d_k + 1 = 2\) in symmetry class AIII lead to the appearance of zero-energy surface flat bands. This is demonstrated in Figs. 3.2(b) and 3.2(c), which show that zero-energy surface states appear in a two-dimensional region of the surface BZ that is bounded by the projection of the nodal ring.

### 3.3 Nodal noncentrosymmetric superconductors

As a second example, we consider nodal noncentrosymmetric superconductors (NCSs). The absence of bulk inversion symmetry in these materials leads to a spin splitting of the electronic bands by spin-orbit coupling. This in
turn allows for the existence of mixed-parity superconducting states with both spin-singlet and spin-triplet pairing components. Over the past few years a number of (nodal) NCSs have been discovered \[68–73\], most notably Li$_2$Pt$_3$B \[58, 74, 75\], BiPd \[76, 77\], and the heavy-fermion compounds CePt$_3$Si \[56, 57, 78, 79\], CeIrSi$_3$ \[80, 81\], and CeRhSi$_3$ \[82\]. Recently, nontrivial topology characteristics of nodal NCSs have been studied both theoretically and experimentally \[37–43, 43, 44, 44–48, 76, 77, 83–86\]. Specifically, it was found that NCSs belong to symmetry class DIII, which according to classification of topologically stable nodal lines in Table 5.3 implies that three-dimensional NCSs can support topologically stable nodal lines. To exemplify the topological features of these nodal superconductors we study in this subsection a simple BdG model Hamiltonian describing a single-band nodal NCSs with monoclinic crystal symmetry $C_2$ (relevant for BiPd). Implications of some of our findings for experiments on BiPd will be discussed at the end of this section.

**Model definition.** We start from the BdG Hamiltonian $H = \frac{1}{2} \sum_k \psi_k^\dagger H(k) \psi_k$, where $\psi_k = (c_{k\uparrow}, c_{k\downarrow}, c_{-k\uparrow}^\dagger, c_{-k\downarrow}^\dagger)\mathrm{^T}$ and

$$H(k) = \begin{pmatrix} h(k) & \Delta(k) \\ \Delta^\dagger(k) & -h^T(-k) \end{pmatrix}.$$  \hspace{1cm} (3.4)

The normal state Hamiltonian

$$h(k) = \epsilon_k \mathbb{I}_{2\times2} + \alpha \vec{l}_k \cdot \vec{\sigma} + \vec{B} \cdot \vec{\sigma},$$  \hspace{1cm} (3.5)

describes electrons hopping on a cubic lattice with dispersion $\epsilon_k = 2t(\cos k_x + \cos k_y + \cos k_z) - \mu$ and Rashba-type antisymmetric spin-orbit coupling $\alpha \vec{l}_k \cdot \vec{\sigma}$. Here, $t$ denotes the hopping amplitude, $\mu$ the chemical potential, $\alpha$ the spin-orbit coupling strength, and $\vec{l}_k = -\vec{l}_{-k}$ the antisymmetric spin-orbit coupling potential. $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)\mathrm{^T}$ represents the vector of Pauli matrices. We have included in Eq. (3.5) a Zeeman term $\vec{B} \cdot \vec{\sigma}$, which allows us to study the stability of the topological surface states against time-reversal symmetry breaking perturbations. The superconducting order parameter $\Delta(k)$ is in general an admixture of even-parity spin-singlet $\Delta_s$ and odd-parity spin-triplet $\Delta_t \vec{d}_k$ components

$$\Delta(k) = \left( \Delta_s \mathbb{I}_{2\times2} + \Delta_t \vec{d}_k \cdot \vec{\sigma} \right) (i\sigma_y).$$  \hspace{1cm} (3.6)

In the following we assume that the spin-triplet pairing vector $\vec{d}_k$ is aligned with the spin-orbit coupling vector $\vec{l}_k$, i.e., we set $\vec{d}_k = \vec{l}_k$. For the numerical computations we will set $(t, \mu, \alpha, \Delta_t) = (-0.5, -2.0, 1.0, 1.0)$. The particular form of $\vec{l}_k$ is constrained by the lattice symmetries of the noncentrosymmetric crystal \[87\]. Within a tight-binding
expansion, we obtain for the monoclinic crystal point group $C_{2}$ to lowest order

$$\vec{l}_k = \begin{pmatrix} a_1 \sin k_x + a_5 \sin k_y \\ a_2 \sin k_y + a_4 \sin k_x \\ a_3 \sin k_z \end{pmatrix}, \quad (3.7)$$

where $a_i$ ($i = 1, \ldots, 5$) are five real parameters.

With the above parametrization, Hamiltonian (3.4) in the absence of a Zeeman magnetic field, i.e. $\vec{B} = 0$, generically exhibits stable nodal lines in the three-dimensional BZ. These nodal lines are in symmetry class DIII (or class AIII if the hypersphere $S_{d^k}$ surrounding the nodal lines is not centrosymmetric), since Hamiltonian (3.4) is invariant under both time-reversal symmetry $T = U_T K$, with $T^2 = -1$, and particle-hole symmetry $P = U_P K$, with $P^2 = +1$. Time-reversal symmetry $T$ acts on the BdG Hamiltonian as

$$U_T^{-1} \mathcal{H}(k) U_T = \mathcal{H}^*(-k), \quad (3.8)$$

where $U_T = \mathbb{I}_{2 \times 2} \otimes i \sigma_2$. Particle-hole symmetry $P$ is implemented as

$$U_P^{-1} \mathcal{H}(k) U_P = -\mathcal{H}^*(-k), \quad (3.9)$$

where $U_P = \sigma_1 \otimes \mathbb{I}_{2 \times 2}$. Observe that upon inclusion of a finite Zeeman magnetic field, $\vec{B} \neq 0$, time-reversal symmetry is broken, whereas particle-hole symmetry remains satisfied. I.e., Hamiltonian (3.4) restricted to $S_{d^k}$ with $\vec{B} \neq 0$ belongs to symmetry class D (or class A if $S_{d^k}$ is not centrosymmetric) and can therefore no longer support stable nodal lines (see Table 5.3).

### 3.3.1 Nodal structures.

The energy spectrum of Eq. (3.4) with $\vec{B} = 0$ is given by $\{-\lambda_{1,k}^-, -\lambda_{2,k}^+, +\lambda_{3,k}^-, +\lambda_{4,k}^+\}$ with $\lambda_k^- = \sqrt{(\xi_k^+)^2 + (\Delta_k^-)^2}$ and $\lambda_k^+ = \sqrt{(\xi_k^-)^2 + (\Delta_k^+)^2}$. Here, we have introduced the shorthand notation $\xi_k^\pm = \varepsilon_k \pm \alpha |\vec{l}_k|$ and $\Delta_k^\pm = \Delta_s \pm \Delta_t |\vec{l}_k|$. Without loss of generality we can take $\Delta_s, \Delta_t > 0$, in which case the positive helicity band $\lambda_k^+$ is always fully gapped, whereas the negative helicity band $\lambda_k^-$ exhibits nodal lines. In Fig. 3.3 we study the nodal structure of the negative helicity band as a function of $\Delta_s$, $a_1 = a_2$, $a_3$, and $a_4 = a_5$. The topological stability of these
nodal rings is guaranteed by the winding number \( \nu_1 \), Eq. (A.15). Using Eqs. (3.4), (3.5), and (3.6) we find that

\[
\nu_1 = \frac{1}{2\pi} \text{Im} \int_{S^1} dk \text{Tr} \left\{ \partial_k \ln \left[ (\varepsilon_k + i\Delta_x) I_{2 \times 2} + (\alpha + i\Delta_x) \ell_k \cdot \sigma \right] \right\},
\]

(3.10)

where \( S^1 \) is a circle in momentum space. For brevity, we discuss only two parameter choices, namely \((\Delta_s, a_1, a_3, a_4) = (1.0, 0.5, 0.0, 0.5) \) [Fig. 3.3(c)] and \((1.8, 0.6, 1.3, 0.6) \) [Fig. 3.3(f)], which we refer to as “Case-1” and “Case-2”, respectively. To determine the topological charges \( \nu_1 \) of the nodal rings for these two cases we consider a noncontractible circle \( S^1 \) along the (100) direction of the BZ torus \( T^3 \). We find that for Case-1 the nodal ring located within the half-space \( k_y > 0 \) of Fig. 3.3(c) carries topological charge \( \nu_1 = +1 \) \((-1) \). For Case-2 the nodal ring in the first and fifth octants of the BZ with \((\text{sgn} k_x, \text{sgn} k_y, \text{sgn} k_z) = (+, +, +) \) and \((+, +, -) \), respectively, have \( \nu_1 = +1 \), whereas the rings in the third and seventh octants with \((\text{sgn} k_x, \text{sgn} k_y, \text{sgn} k_z) = (-, -, +) \) and \((-,-,-) \), respectively, have \( \nu_1 = -1 \).

### 3.3.2 Surface band structure.

Due to the bulk-boundary correspondence of Sec. 5.2.5 the topologically nontrivial nodal lines of Hamiltonian (3.4) give rise to zero-energy surface flat bands. That is, zero-energy states appear within two-dimensional

\[^3\text{In certain cases, provided that } S^1 \text{ is centrosymmetric, the stability of the nodal lines is also protected by the } \mathbb{Z}_2 \text{ number } W_1, \text{ Eq. (A.21), see Refs. [40][42].}\]
regions of the surface BZ that are bounded by the projected bulk nodal lines. This is illustrated in Fig. 3.4 which shows the surface band structure of Hamiltonian (3.4) on the (100) and (001) faces. On the (100) face, the projected nodal rings for both Case-1 and Case-2 do not overlap leading to several zero-energy surface flat bands [see Figs. 3.4(a) and 3.4(d)]. Similar considerations also hold for the (010) surface, since for the considered parameter choices the absolute value of the spin-orbit coupling vector $|\vec{l}_k|$ is symmetric under the interchange of $k_x$ with $k_y$. On the (001) face for Case-2, on the other hand, two projected nodal rings with opposite topological charge overlap, and hence the two topological charges cancel. Consequently, there are no flat-band states appearing on the (001) face for Case-2 [see Fig. 3.4(e)]. This is in fact a generic property of model (3.4). Since $|\vec{l}_k|$ is symmetric under $k_z \rightarrow -k_z$, the topological charges of the projected nodal rings in the surface BZ of the (001) face always add up to zero. Hence, there are no zero-energy flat bands appearing on the (001) surface, irrespective of the parameter choice for $\vec{l}_k$, Eq. (3.7).

In Figs. 3.4(b) and 3.4(c) we study how the surface band structure on the (100) face for Case-1 is modified in the presence of a time-reversal symmetry breaking Zeeman field $\vec{B} \neq 0$. Interestingly, we find that a field along the $z$-axis leaves the flat bands unaffected [Fig. 3.4(b)], whereas a field within the $x - y$ plane gives rise to an energy shift of the flat-band states [Figs. 3.4(c)]. This behavior can be explained in terms of the strong spin polarization of the flat-band states. It turns out that the surface flat bands of Fig. 3.4(a) are spin polarized within the $x - y$ plane, and consequently

\footnote{Remember that the topological charge of a given nodal ring depends on the chosen integration path $S^1$ in Eq. (3.10). Consequently, the topological charge of a projected nodal ring in the surface BZ depends on the surface orientation.}
3.3.3 Surface density of states.

Surface flat bands manifest themselves as a zero-energy divergence in the surface density of states, and hence give rise to a zero-bias peak in the tunneling conductance [41, 42]. This zero-bias conductance peak depends strongly on the surface orientation, due to the changing projection of the bulk nodal rings onto the surface BZ. To illustrate this dependence, let us compute the surface density of states of the noncentrosymmetric superconductor (3.4). The density of states in the \( x \)-th layer from, e.g., the (100) surface is given by

\[
D(x, E) = \frac{1}{N_y N_z} \sum_{n,k_{\parallel}} \left[ (|v_{n\uparrow}(x, k_{\parallel})|^2 + |v_{n\downarrow}(x, k_{\parallel})|^2) \delta(E - E_n(k_{\parallel})) \\
+ (|u_{n\uparrow}(x, k_{\parallel})|^2 + |u_{n\downarrow}(x, k_{\parallel})|^2) \delta(E + E_n(k_{\parallel})) \right],
\]

(3.11)

where \( k_{\parallel} = (k_y, k_z) \) represents the surface momenta, \( N_y \) and \( N_z \) are the number of \( k_y \) and \( k_z \) points, respectively, in the surface BZ, and \( \phi_n(x, k_{\parallel}) = (u_{n\uparrow}(x, k_{\parallel}), u_{n\downarrow}(x, k_{\parallel}), v_{n\uparrow}(x, k_{\parallel}), v_{n\downarrow}(k_{\parallel})) \) denotes the eigenvector of \( \mathcal{H}(x, x', k_{\parallel}) = \frac{1}{2\pi} \int dk_x e^{ik_x(x-x')} \mathcal{H}(k) \) with eigenenergy \( E_n(k_{\parallel}) \), i.e., \( \mathcal{H}(x, x', k_{\parallel})\phi_n(x', k_{\parallel}) = E_n(k_{\parallel})\phi_n(x, k_{\parallel}) \).

Fig. 3.5 displays the surface density of states \( D(x = 1, E) \) at the (100) face of \( \mathcal{H}(k) \) for the parameter choice Case-1, both in the presence and in the absence of an external magnetic field \( \vec{B} \). While a field along the \( z \)-axis does not split the zero-energy peak (Figs. 3.5(b) and (c)), we find that a field with a finite component in the \( x - y \) plane leads to a splitting which is roughly proportional to the field strength \( |\vec{B}| \) [Fig. 3.5(d), cf. also Figs. 3.4(c)].

3.3.4 Implications for experiments on BiPd.

BiPd is a NCS with transition temperature \( T_C = 3.8 \) K [76]. Recently, a zero-bias conductance peak in point contact measurements of BiPd single crystals has been reported [77]. Due to the large number of atoms in its unit...
cell, BiPd has low crystal symmetry, with monoclinic point group $C_2$ and no center of inversion. Moreover, bismuth has a high atomic number, which gives rise to strong spin-orbit coupling. These two properties together likely lead to multiple spin-split Fermi surfaces and, correspondingly, to a superconducting state with multigap character. It is not unlikely that at least one of these multiple gaps has nontrivial topological properties.

Even though the simple single-band Hamiltonian (3.4) shares the same point group symmetry $C_2$ with BiPd, it only provides a very crude model for this NCS. An accurate phenomenological description of BiPd would require detailed knowledge of the band structure, the pairing symmetry, and the pairing mechanism of this superconductor. In the absence of this information, we can only speculate about possible origins of the zero-bias conductance peak observed in BiPd. According to Ref. [77], one plausible explanation is that BiPd is a nodal topological superconductor with zero-energy surface flat bands. A pronounced zero-bias conductance peak has been observed for contacts both on the (010) face and on the (001) face, although in the latter case the intensity is somewhat weaker [77]. While the zero-bias peak for the (010) surface is in agreement with Hamiltonian (3.4), the conductance peak for the (001) face cannot be explained within this simple model description (see discussion on page 15). The source of this discrepancy probably lies in the oversimplified assumptions made for the band structure and gap functions entering in model (3.4). Impurity scattering and interface roughness are further complications that need to be taken into account when interpreting the interesting point contact conductance measurements of Ref. [77].

### 3.4 Robustness of surface flat bands against disorder

Determining the robustness of gapless topological phases and their topological surface states against disorder requires a careful analysis of different types of scattering processes involving both quasiparticle bulk and surface states. How susceptible any topological Fermi surface is to impurity effects crucially depends on symmetry properties and on their codimension $q$. The latter follows, for instance, from a simple renormalization group argument which shows that uncorrelated (or short-range) correlated on-site disorder is marginal by power counting for Fermi surfaces with $q = 2$ and irrelevant for Fermi surfaces with $q > 2$. Since a detailed analysis of disorder effects in gapless topological phases is beyond the scope of this section, we focus here on impurity effects, mostly in nodal NCSs [cf. Sec. 3.3], and only briefly discuss some general arguments suggesting that the surface flat bands of these systems are partly protected against disorder.

(i) First, we observe that similar to other topological systems with strong spin-orbit interactions [3][6], the surface states of NCSs possess a helical spin texture [84][85]. That is, the surface flat bands are strongly spin polarized, with states with opposite momenta exhibiting opposite spin polarization. This nontrivial spin texture leads to the absence (or suppression) of nonmagnetic scattering processes connecting states with opposite (or nearly opposite) spin
polarization. Moreover, impurity scattering processes coupling zero-energy surface states to bulk nodal quasiparticles are suppressed, due to the vanishing bulk density of states at zero energy.

(ii) Second, we note that the topological charge (e.g., Eq. (A.13)) can be defined also for gapless topological states with dilute impurities, for example, by periodically repeating a finite-size disordered system. Such an approach shows that the topological number of a disordered nodal NCSs remains nonzero for a large set of quasi-momenta. In passing, we mention that this method has recently been applied to study zero-energy edge states in graphene in the presence of edge disorder [88, 89].

(iii) Third, we discuss the role played by symmetries which restrict the form of the impurity potential. In particular, chiral symmetry (sublattice symmetry) usually prohibits a large number of scattering channels. For example, for two-dimensional nodal topological superconductors in symmetry class BDI [90] (and also for graphene [91, 92]), it was shown that on a given edge all localized zero-energy states have the same chirality number, i.e., all zero-energy edge states are simultaneous eigenstates of the chiral symmetry operator $S$ with the same eigenvalue $+1$ (or $-1$). Since on-site impurities do not break chiral symmetry, the total chirality number of a given edge remains unchanged in the presence of impurities, and hence the total number of zero-energy edge states is not altered by disorder. For noncentrosymmetric superconductors (Sec. 3.3), on the other hand, chiral symmetry is less restrictive, since on a given surface there are zero-energy states with both chirality numbers, $+1$ and $-1$.

In summary, the above arguments suggest that the zero-energy surface states of gapless topological phases are at least partially robust against disorder. A more detailed investigation of the influence of disorder on the topological surface states is left for future work.
Chapter 4

Majorana vortex-bound states in three-dimensional nodal noncentrosymmetric superconductors

4.1 Introduction

Topological superconductors have in recent years become a subject of intense research due to their potential use for technical applications in device fabrication and quantum information [3, 4, 6, 93]. By the bulk-boundary correspondence, zero-energy Majorana modes appear at the surface or inside the vortex core of topological superconductors. The experimental search for Majorana modes, which can be utilized as basic building blocks (i.e., half a qubit) for topological quantum computers, is the focus of a growing research effort [94–97]. These Majorana modes are robust against symmetry preserving impurity scattering processes and deformations of the superconducting order parameter. While topological superconductivity can be artificially engineered in heterostructures with an ordinary $s$-wave superconductor and, say, a semiconductor [98–100] or a topological insulator [8], it can also occur naturally in certain correlated materials with strong spin-orbit coupling (SOC).

One promising class of materials for topological superconductivity are the noncentrosymmetric superconductors (NCSs) [68]. In these systems, the absence of inversion symmetry together with strong SOC and electronic correlations can give rise to unconventional pairing states with topologically nontrivial characteristics [38–44, 46, 47, 101]. For example, in CePt$_3$Si [56, 57, 78, 79], macroscopic as well as microscopic measurements indicate an unconventional superconducting state with a mixture of spin-singlet and spin-triplet pairing components and line nodes in the superconducting gap. Experimental evidence for unconventional pairing symmetries has also been reported for CeIrSi$_3$ [80, 81], CeRhSi$_3$ [82], Y$_2$C$_3$ [102], Li$_2$Pt$_3$B [58, 74, 75], and BiPd [76, 77]. Both fully gapped and nodal NCSs with sizable spin-triplet pairing components exhibit nontrivial topological properties, which manifest themselves in terms of different types of zero-energy surface states. In fully gapped NCSs the surface states are dispersing helical Majorana modes, whereas nodal NCSs exhibit surface flat bands [38, 40, 44, 45, 47], and depending on the crystallographic point group, may also support helical Majorana modes or surface arc states [42]. Experimentally, it is possible to distinguish among different types of surface states using Fourier-transform scanning tunneling spectroscopy [103] or surface transport measurements [84, 104].

Most of the candidate materials for noncentrosymmetric topological superconductivity are strong type-II super-
conductors, with Ginzburg-Landau parameters $\kappa$ of the order of $\sim 100$ \cite{68}. Hence, zero-energy Majorana modes may emerge inside magnetic vortices of these superconducting compounds \cite{38,105,107}. In this chapter, we examine vortex-bound states of three-dimensional (3D) NCSs and study how their appearance is related to the crystal point-group symmetries of the superconductor and the nontrivial topological properties of the bulk Bogoliubov-quasiparticle wave functions. Using both numerical and analytical methods, we compute the vortex-bound state spectra of $(s + p)$-wave NCSs with three different point-group symmetries: the two tetragonal point-groups $D_4$ and $C_{4v}$, as well as the monoclinic point-group $C_{2h}$.

One of our primary findings is that $D_4$ point-group NCSs support gapless helical Majorana states inside vortex cores. These subgap states disperse linearly along the vortex line, and are akin to one-dimensional helical Majorana modes that exist at the edge of fully gapped topological NCSs in two dimensions. Remarkably, these vortex-bound states appear both in the fully gapped topological phase and in the nodal phase that separates the fully gapped trivial phase from the topological one [see Figs. 4.1(a) and 4.2]. While these helical Majorana vortex states exist in an extended region of the phase diagram of Fig. 4.1(a), they are unstable against perturbations that break the $D_4$ point-group symmetry of the superconductor (SC). For NCSs with tetragonal point-group symmetry $C_{4v}$, on the other hand, we find that there are zero-energy vortex-bound states which are dispersionless along the vortex line, forming a one-dimensional Majorana flat band [Fig. 4.3]. In contrast, $C_2$ point-group NCSs do not exhibit any zero-energy vortex-bound states neither in the fully gapped nor in the nodal phase [Fig. 4.4]. We find that the Majorana vortex-bound states of the $C_{4v}$ ($D_4$) point-group NCS are protected by a combination of reflection ($\pi$ rotation), time-reversal, and particle-hole symmetry.

Interestingly, the existence of these vortex-bound states in nodal NCSs correlates to some degree with the appearance of extra surface states, that appear in addition to the surface flat bands. That is, for nodal NCSs with $D_4$ point-group symmetry the helical vortex-bound states always appear together with helical Majorana cones on the surface which are protected by a $\mathbb{Z}_2$ topological number \cite{40,42}. (In the following, we refer to these Majorana cone surface states as the “$\mathbb{Z}_2$ surface states.”) On the other hand, for nodal $C_{4v}$ point-group NCSs the existence of flat-band vortex states is correlated with the appearance of helical arc states on the surface \cite{42}, see Table 6.1. These surface arc states are superconducting analogues of the Fermi arcs that exist on the surface of Weyl semimetals \cite{24,26} [see Sec. 2.2]. Using translation symmetry in the vortex direction, we fix the momentum along the vortex line and consider adiabatic deformations of the quasiparticle spectrum that do not close the bulk energy gap for this fixed momentum. By use of this procedure, we find that the vortex-bound states (extra surface states) of $D_4$ and $C_{4v}$ point-group NCSs are adiabatically connected to the vortex-bound states (surface states) of fully gapped topological SCs and time-reversal

\footnote{For previous studies on stable Majorana vortex-bound states in fully gapped 2D NCSs, in 3D SCs with Rashba-spin orbit coupling, and NCSs with cubic crystal symmetry $O$, see Refs. \cite{46,105,107}.}

\footnote{This is in some sense expected since helical modes are unstable against TRS breaking perturbation, and here vortices break TRS.}
symmetric Weyl SCs, respectively. Conversely, finite-energy vortex-bound states of nodal NCSs with $C_2$ point-group symmetry can be related to finite-energy vortex-bound states of fully gapped trivial SCs [cf. Table 6.1].

### 4.2 Model Hamiltonian and symmetries

To study the appearance of vortex-bound states in nodal NCSs, we consider a generic single-band Bogoliubov-de Gennes (BdG) Hamiltonian $H = \sum_{k \in BZ} \Psi_k^\dagger \mathcal{H}(k) \Psi_k$, with

$$
\mathcal{H}(k) = \begin{pmatrix}
h(k) & \Delta(k) \\
\Delta^\dagger(k) & -h^T(-k)
\end{pmatrix},
$$

(4.1)

and the Nambu spinor $\Psi_k = (c_{k\uparrow}, c_{k\downarrow}, c_{-k\uparrow}^\dagger, c_{-k\downarrow}^\dagger)^T$, where $c_{k\sigma}$ ($c_{k\sigma}^\dagger$) denotes the electron annihilation (creation) operator with momentum $k$ and spin $\sigma = \uparrow, \downarrow$. The normal-state Hamiltonian $h(k) = \varepsilon(k) \mathbb{I}_{2 \times 2} + \alpha \mathbf{l}(k) \cdot \sigma$ describes electrons on a cubic lattice with nearest-neighbor hopping $t$, chemical potential $\mu$, spin-independent dispersion $\varepsilon(k) = t(\cos k_x + \cos k_y + \cos k_z) - \mu$, and Rashba-type SOC $\mathbf{a}(\mathbf{l}(k) \cdot \sigma) (i \sigma_2)$, where $\Delta_s$ and $\Delta_t$ represent the spin-singlet and spin-triplet pairing amplitudes, respectively. For the spin-triplet pairing term we assume that the vector $\mathbf{d}(k)$ is oriented parallel to the polarization vector $\mathbf{l}(k)$ of the SOC [108].

To simplify matters we will set $(t, \alpha, \Delta_t) = (-1, 1, 1)$ in our numerical calculations and study the vortex-bound states as a function of $\Delta_s$, $\mu$, and different types of SOC potentials. We have checked that different values of $(t, \alpha, \Delta_t)$ do not qualitatively change our results. With $\varepsilon(k) = \varepsilon(-k)$ and $\mathbf{l}(k) = -\mathbf{l}(-k)$, Hamiltonian (4.1) is invariant under both time-reversal symmetry (TRS) and particle-hole symmetry (PHS),

$$
U_T^{-1} \mathcal{H}(k) U_T = \mathcal{H}^*(-k)
$$

(4.2a)

and

$$
U_P^{-1} \mathcal{H}(k) U_P = -\mathcal{H}^*(-k),
$$

(4.2b)

where $U_T = \mathbb{I}_{2 \times 2} \otimes i \sigma_2$ and $U_P = \sigma_1 \otimes \mathbb{I}_{2 \times 2}$, respectively. Hence, since $U_T U_T^+ = -\mathbb{I}_{4 \times 4}$ and $U_P U_P^+ = \mathbb{I}_{4 \times 4}$, $\mathcal{H}(k)$ belongs to symmetry class DIII.

The specific form of the spin-orbit coupling vector $\mathbf{l}(k)$ is constrained by the lattice symmetries of the superconductor [87]. In the following we consider NCSs with three different crystal point-group symmetries: the tetragonal
Table 4.1: Depending on the crystal point-group symmetries (first column), nodal NCSs can exhibit different types of zero-energy vortex-bound states (second column). As indicated in the third column, the appearance of these different vortex states correlates with the existence of extra surface states besides the flat-band states. The helical vortex states and the $\mathbb{Z}_2$ surface states of nodal $D_4$ NCSs can be adiabatically connected to the vortex-bound and surface states of fully gapped topological NCSs. Similarly, the flat-band vortex states and arc surface states of $C_{4v}$ NCSs are related to the vortex-bound and surface states of time-reversal symmetric Weyl SCs.

<table>
<thead>
<tr>
<th>Point Group</th>
<th>Vortex States</th>
<th>Extra Surface States</th>
<th>Adiabatic Deformation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_4$</td>
<td>helical states</td>
<td>$\mathbb{Z}_2$ Majorana cone</td>
<td>fully gapped top. SC</td>
</tr>
<tr>
<td>$C_{4v}$</td>
<td>flat bands</td>
<td>helical arc states</td>
<td>Weyl SC with TRS</td>
</tr>
<tr>
<td>$C_2^\perp$</td>
<td>none</td>
<td>none</td>
<td>gapped trivial SC</td>
</tr>
</tbody>
</table>

* for phase IV in Fig. 1(c).

point groups $D_4$ and $C_{4v}$, as well as the monoclinic point group $C_2$. Within a tight-binding expansion, we obtain for the crystal point group $D_4$ to lowest order

$$I(k) = (a_1 \sin k_x, a_1 \sin k_y, a_2 \sin k_z).$$

(4.3a)

For the tetragonal point group $C_{4v}$, which is relevant for CePt$_3$Si, CeRhSi$_3$, and CeIrSi$_3$, the vector $I(k)$ takes the form

$$I(k) = a_1(\sin k_y, -\sin k_x, 0).$$

(4.3b)

The lowest order terms compatible with $C_2$ point-group symmetry (represented by BiPd) are given by

$$I(k) = (a_1 \sin k_x + a_5 \sin k_y, a_2 \sin k_y + a_4 \sin k_x, a_3 \sin k_z).$$

(4.3c)

$D_4$ and $C_{4v}$ NCSs exhibit, besides the global symmetries TRS and PHS, also rotation and reflection symmetries. Two of these crystalline symmetries play an important role for the protection of zero-energy vortex-bound states. Let us discuss these in more detail. We find that the $D_4$ NCS is invariant under $\pi$ rotation along the $x$ axis, which acts on the Hamiltonian (4.1) as

$$U_{R_\pi}^\dagger \mathcal{H}(R_\pi k)U_{R_\pi} = \mathcal{H}(k),$$

(4.4)

where $U_{R_\pi} = \text{diag}(u_{R_\pi}, u_{R_\pi}^*)$ and $u_{R_\pi}$ is the spinor representation of the rotation $R_\pi = \text{diag}(1, -1, -1)$, i.e.,

$$u_{R_\pi} = \exp[-i(\pi/2)\sigma_1] = -i\sigma_1.$$

The $C_{4v}$ point-group NCS, on the other hand, satisfies the reflection symmetry

$$U_{R_y}^\dagger \mathcal{H}(R_y k)U_{R_y} = \mathcal{H}(k),$$

(4.5)

23
with \( U^\dagger_{R_y} = \text{diag}(u^*_{R_y}, u_{R_y}) \) and \( u_{R_y} = i\sigma_2 \) the spinor representation of the reflection operator \( R_y = \text{diag}(1, -1, 1) \).

For a pair of vortex-antivortex lines oriented along the \( z \)-axis, the spin-singlet and spin-triplet order parameters are modified as

\[
\Delta_{s,t}(x, y) = \Delta_{s,t} e^{i\phi(x, y)},
\]

where the phase angle \( \phi(x, y) \) is given by \( \phi(x, y) = \arctan\left(2aby/(x^2 + (by)^2 - a^2)\right) \). This describes a vortex and antivortex line with winding number \( \pm 1 \) located at \( (a, 0) \) and \( (-a, 0) \), respectively. The anisotropy of the vortex line is controlled by the parameter \( b \). In order to compute the vortex-bound states we set \( (a, b) = (8, 2) \) and diagonalize the BdG Hamiltonian (4.1) on a \( 50 \times 50 \times 60 \) cubic lattice with periodic boundary conditions (PBCs) in all three directions. To simplify matters, we do not take into account the Zeeman effect. Most NCS topological superconductor candidate materials are extreme type-II superconductors\[^68\] with a lower critical field \( H_{c1} \) of the order of 1 mT, corresponding to an energy scale an order of magnitude smaller than the gap energy. For these systems, it is expected that the Zeeman effect can be neglected for a magnetic field that is not much larger than \( H_{c1} \).

The Hamiltonian in the presence of a pair of vortex-antivortex lines along the \( z \)-axis breaks TRS as well as the crystal symmetries (4.4) and (4.5), but remains invariant under a combination of TRS with crystal symmetries. That is, the \( D_4 \) point-group NCS with \( k_z = 0 \) satisfies the following symmetry

\[
[U_{R_x} U_T]^{-1} \tilde{\mathcal{H}}(x, x', y, y') [U_{R_x} U_T] = \tilde{\mathcal{H}}^*(x, x', y, y'), \quad (4.7a)
\]

where \( \tilde{\mathcal{H}}(x, x', y, y') \) denotes the Fourier transform of \( \mathcal{H}(k_x, k_y, k_z = 0) \), \( U_{R_x} = \delta_{x,x} \delta_{y,-y} U_{R_x} \) is the real-space \( \pi \)-rotation operator, and \( U_T = \delta_{x,x} \delta_{y,y} \otimes U_T \) represents the time-reversal operator in position space. Similarly, for the \( C_{4v} \) NCS in the presence of vortices, we find the following symmetry

\[
[U_{R_y} U_T]^{-1} \tilde{\mathcal{H}}(x, x', y, y', k_z) [U_{R_y} U_T] = \tilde{\mathcal{H}}^*(x, x', y, y', k_z), \quad (4.7b)
\]

for all \( k_z \), where \( U_{R_y} = \delta_{x,x} \delta_{y,-y} \otimes U_{R_y} \) denotes the reflection operator in real space. Here, the matrix \( \delta_{x,x} \delta_{y,-y} \) acts on the real-space basis, while \( U_{R_y} \) acts on the Nambu basis. We note that the \( C_2 \) NCSs does not possess any symmetry of the form of Eqs. (4.7). In Sec. 4.4 it is shown that symmetries (4.7) together with PHS lead to the protection of zero-energy vortex-bound states.
4.3 Phase diagram and topological invariants

The phase diagram of Hamiltonian (4.1) in the absence of vortices is shown in Figs. 4.1(a)-4.1(c) as a function of spin-singlet pairing amplitude $\Delta_s$ and chemical potential $\mu$. Two fully gapped phases with trivial and nontrivial topology [phases I and II in Fig. 4.1] are separated by a nodal superconducting phase [phases III and IV in Fig. 4.1].

Interestingly, for the $C_2$ point-group NCS we find that there are two distinct gapless phases with a Lifshitz transition in between, at which the nodal rings touch each other and reconnect in a different manner [see Figs. 4.1(d) and 4.4(a)-4.4(d)]. The topological properties of the fully gapped phases I and II in Fig. 4.1 are characterized by the 3D winding number $\nu_3$ which is defined as

$$\nu_3 = \int_{BZ} \frac{d^3k}{24\pi^2} \epsilon^{\mu\nu\rho} \text{Tr}[(q^{-1}\partial_{k_\mu} q)(q^{-1}\partial_{k_\nu} q)(q^{-1}\partial_{k_\rho} q)],$$

where $q$ is the off-diagonal block of the spectral projector, see Appendix A.1.2. We find that phase I is topologically nontrivial with $\nu_3 = -1$, while phase II is trivial with $\nu_3 = 0$. Note that this 3D winding number $\nu_3$ is only well defined for fully gapped phases. The topological characteristics of the nodal phases III and IV, however, can be described by the one-dimensional winding number $\nu_1$ [40, 47]

$$\nu_1 = \frac{i}{2\pi} \oint L \, dk_\mu \, \text{Tr}[q^{-1}\partial_{k_\mu} q],$$

where $L$ is a closed path that interlinks with a line node. In both nodal phases III and IV, the winding number $\nu_1$ evaluates to $\pm 1$ for each nodal ring. To characterize the nodal phases it is also possible to define a one- or two-dimensional $\mathbb{Z}_2$ topological invariant $[40, 47]$ [see App. A.1.2]

$$W_A = \prod_{\kappa} \frac{\text{Pf} \left[ q^T(K) \right]}{\sqrt{\det \left[ q(K) \right]}},$$

where $A$ is a time-reversal invariant line or plane embedded in the 3D Brillouin zone (BZ) and $K$ denotes the two (four) time-reversal invariant momenta on the line (plane) $A$.

4.4 Vortex-bound states and surface states

In this section we discuss the surface states and vortex-bound states of nodal NCS with the three different point-group symmetries $D_4$, $C_{4v}$, and $C_2$.\footnote{The gap closes when $0 = |B - A||l|$ with $B = \epsilon(k) + i\Delta_s$ and $A = \alpha + i\Delta_t$. The gapless points are the intersections between hypersurfaces that are characterized by these two equations: $t(\cos k_x + \cos k_y + \cos k_z) = \mu + \alpha \Delta_s/\Delta_t$ and $|l| = \Delta_s/\Delta_t$.}
Figure 4.1: Phase diagram of Hamiltonian (4.1) as a function of spin-singlet pairing amplitude $\Delta_s$ and chemical potential $\mu$ for the point group (a) $D_4$ with $(a_1, a_2) = (1.0, 0.3)$, (b) $C_4v$ with $a_1 = 1.0$, and (c) $C_2$ with $(a_1 = a_2, a_3, a_4 = a_5) = (1.0, 0.3, 0.5)$. The fully gapped phases (red shaded regions) are characterized by the winding number $\nu_3$, where $\nu_3 = -1$ (phase I) corresponds to the topological phase, while $\nu_3 = 0$ (phase II) is the trivial phase. The blue dashed line in panel (c) represents the phase boundary between the two distinct nodal structures III and IV shown in panel (d).

4.4.1 $D_4$ point-group NCSs

We start by considering a nodal NCS with $D_4$ point-group symmetry in phase III of Fig. 4.1(a). In this region of parameter space the bulk Bogoliubov quasiparticle spectrum exhibits two topologically stable nodal rings, which are centered about the (001) axis [Figs. 4.2(a) and 4.2(b)]. The one-dimensional winding number $\nu_1$ (topological charge) of these two nodal rings is $\nu_1 = \pm 1$, which by the bulk-boundary correspondence results in the appearance of flat-band surface states [40, 42]. In addition to the surface flat bands, nodal $D_4$ NCSs exhibit $\mathbb{Z}_2$ Majorana surface states. This is shown in Figs. 4.2(c) and 4.2(d) for the (100) surface, where a helical Majorana cone appears at $(k_y, k_z) = (0, 0)$ of the surface BZ. As shown in Ref. [40], this Majorana surface state is protected by the one-dimensional $\mathbb{Z}_2$ topological invariant (4.10) with $\mathcal{A}$ a time-reversal invariant line. Choosing $\mathcal{A}$ to be oriented along the $k_x$ axis with $(k_y, k_z)$ held fixed, we find that $W_{\mathcal{A}} = -1$ at $(k_y, k_z) = (0, 0)$, which signals the appearance of a zero-energy helical Majorana state. At the other three time-reversal invariant momenta of the surface BZ there are no surface states, in agreement with $W_{\mathcal{A}} = +1$ for these surface momenta.

$D_4$ point-group NCSs support zero-energy helical Majorana states not only on the surface but also inside vortex cores. This is illustrated in Fig. 4.2(e), which shows the energy spectrum in the presence of a pair of vortex and antivortex lines oriented along the $z$ axis. At energies smaller than the bulk gap there appear vortex-bound states which
disperse linearly along the vortex lines. These vortex-bound states are similar to the one-dimensional helical Majorana modes that exist at the edge of a fully gapped topological NCS in two dimensions. The numerical simulations of Fig. 4.2 are in excellent agreement with an analytical derivation of the vortex-bound states, cf. Appendix B.1 and Ref. [105].

The zero-energy vortex-bound states at \( k_z = 0 \) are protected by a combination of \( \pi \) rotation, time-reversal, and particle-hole symmetry; see Eq. (4.7a) [109–111]. Namely, we find that these zero energy modes are eigenstates of the chiral operator \( S = U_R U_I U_P \) and their stability is guaranteed by the conservation of chiral symmetry. That is, the doubly degenerate zero energy states at the vortex core are eigenstates of \( S \) with eigenvalue +1, whereas the two zero-energy modes at the anti-vortex have eigenvalues -1. Without breaking chiral symmetry, a zero-energy state in the vortex core with chirality eigenvalue +1 can only be removed together with a zero mode at the anti-vortex with chirality -1. Hence, in the limit where vortex and anti-vortex cores are separated by a large distance, the zero-energy vortex-bound states are robust against any local perturbation that does not break chiral symmetry \( S \). In particular, the zero-energy vortex-bound states remain unperturbed by the chiral symmetric Zeeman field \( h_z \sigma_z \otimes \sigma_z \).

By employing continuous deformations of the quasiparticle spectrum of Hamiltonian (4.1), one can show that the \( \mathbb{Z}_2 \) surface states and the helical vortex-bound states of the nodal NCS with \( D_4 \) point-group symmetry [phase III in Fig. 4.1(a)] originate from the nontrivial properties of the adjacent fully gapped phase of the \( D_4 \) NCS [phase I in Fig. 4.1(a)]. To be more specific, let us fix the momentum along the vortex line (e.g., to \( k_z = 0 \)) and consider adiabatic deformations connecting phase III to phase I that do not close the bulk gap at this particular momentum. During this deformation process, the two nodal rings shrink to nodal points at the north and south poles of the Fermi sphere and vanish, while the zero-energy vortex and surface states at \( k_z = 0 \) remain unaffected. Moreover, the \( \mathbb{Z}_2 \) invariant \( W_A \) of the nodal phase III can be shown to be directly related to the 3D winding number \( \nu_3 \) of the fully gapped phase I (cf. Ref. [46]). Hence, the zero-energy vortex and \( \mathbb{Z}_2 \) surface states of a nodal \( D_4 \) NCS are adiabatically connected to the vortex and surface states of a fully gapped topological NCS with \( D_4 \) point-group symmetry. A similar deformation process connecting phase III to phase II, on the other hand, does not exist, since upon crossing the transition line between phase III and phase I, the nodal rings approach each other and pair-annihilate. As a result, the zero-energy \( \mathbb{Z}_2 \) surface states and vortex-bound states disappear as one traverses the transition line.

\[^4\]Following Ref. [105], we consider the normal state band structure \( h = ( - \frac{\nabla^2}{2m} - \mu ) \mathbb{I}_{2 \times 2} + \alpha I(k) \cdot \sigma \) and the pairing term \( \Delta = ( \Delta_s + \frac{i}{2} \nabla \cdot D \cdot \nabla ) \mathbb{I}_{\sigma_2} \). We can introduce a vortex line along the \( z \) axis localized at the origin by adding a phase on gap functions for both singlet and triplet pairings. In the continuum model, we need to linearize \( I(k) = (a_1 k_x, a_1 k_y, a_3 k_z) \). In addition, we consider the asymptotic limit \( (1/r \to 0) \) that we can neglect all \( \frac{1}{r} \) and \( \frac{1}{r^2} \) terms in the continuum BdG equation, where \( r \) is the radial direction in the cylindrical coordinate. As the result, there is a localized zero energy solution that decays as a function of \( r \).
Figure 4.2: Zero-energy vortex-bound states and surface states in a D$_4$ point-group NCS with $(a_1, a_2) = (1.0, 0.3)$, $\mu = -2.5$, and $\Delta_s = 0.5$. This parameter choice corresponds to phase III in Fig. 4.1(a). Energies are measured in the unit of hopping. (a) Bulk nodal structure. (b) and (c): Energy spectrum in the absence of vortices as a function of $k_z$ with (b) PBCs in all three directions and (c) OBCs along the $x$ axis but PBCs in the other two directions. (d) Energy dispersion of the highest negative-energy state of the $D_4$ NCS in a (100) slab geometry. The color scale is such that white represents zero energy. (e) Energy spectrum as a function of $k_z$ in the presence of a vortex-antivortex pair oriented along the $z$ axis. The subgap states are localized at the vortex cores. (f) Probability distribution of the zero-energy vortex-bound states as a function of lattice position.

4.4.2 C$_{4v}$ point-group NCSs

Next we study surface and vortex-bound states of a nodal C$_{4v}$ point-group NCS in phase III of Fig. 4.1(b). The bulk quasiparticle spectrum in this nodal phase [Figs. 4.3(a) and 4.3(b)] resembles the one of the $D_4$ NCS [Figs. 4.2(a) and 4.2(b)] and shows two nodal rings around the poles of the Fermi sphere. These line nodes have a nontrivial topological charge, which, as a consequence of the bulk-boundary correspondence, lead to the appearance of flat-band surface states. In addition, C$_{4v}$ NCSs support helical arc surface states, that connect the projected nodal rings in the surface BZ [see Figs. 4.3(c) and 4.3(d)]. These helical arc surface states are protected by a two-dimensional $\mathbb{Z}_2$ number, which is defined for each plane perpendicular to the (001) direction, (i.e., for planes with fixed $k_z$) [42], see Appendix B.2. The arc surface states of C$_{4v}$ NCSs can be viewed as superconducting analogues of the Fermi arcs in time-reversal symmetric Weyl semimetals [31, 112], or alternatively as time-reversal invariant versions of the arc states in the A phase of superfluid $^3$He [21, 61].

Due to the bulk-vortex correspondence [21], vortex lines in C$_{4v}$ NCSs support zero-energy bound states which are...
Figure 4.3: Same as Fig. 4.2 but for a $C_4v$ point-group NCS with $a_1 = 1.0$, $\mu = -2.5$, and $\Delta_s = 0.5$, corresponding to phase III in Fig. 4.1(b).

dispersionless along the vortex line. This is illustrated in Figs. 4.3(e) and 4.3(f) for a pair of vortex and antivortex lines that are oriented along the $z$ axis. Just as the arc surface states, these flat-band vortex-bound states connect the projected bulk nodes in $k_z$ momentum space. Following similar arguments as in Sec. 4.4.1, it can be shown that the zero-energy vortex-bound states of the $C_4v$ NCSs for any fixed $k_z$ are protected by the chiral symmetry $S = U_{R\mu}U_TU_P$; see Eq. (4.7b). Using an adiabatic deformation of the Bogoliubov quasiparticle spectrum that does not close the bulk energy gap at the momenta $k_z$ in between the two projected nodal rings, we find that the flat-band vortex states and the arc surface states of the $C_4v$ NCSs can be related to the vortex states and surface states of a time-reversal symmetric Weyl superconductor. That is, upon approaching the boundary of phase III in Fig. 4.1(b) where $\Delta_s = 0$ and $\mu > -3$, the nodal rings shrink to points at the north and south poles of the Fermi sphere and the $C_4v$ NCSs turns into a time-reversal invariant Weyl superconductor, i.e., a time-reversal symmetric analog of the A phase of $^3$He.

**4.4.3 $C_2$ point-group NCSs**

Lastly, we examine the surface and vortex-bound states of NCSs with $C_2$ point-group symmetry. The phase diagram of $C_2$ NCSs as a function of spin-singlet pairing amplitude $\Delta_s$ and chemical potential $\mu$ displays two distinct nodal phases, which differ in the orientation of the nodal rings [Figs. 4.1(c), 4.1(d), and 4.4(a)-4.4(d)]. In phase III the nodal rings are oriented along the (001) axis, while in phase IV they are centered about the (110) direction. As in the previous two cases, the topological characteristics of these nodal rings, which is described by the one-dimension
Figure 4.4: (Color online). Bulk nodal structure, surface states, and finite-energy vortex-bound states for a $C_2$ point-group NCS with $a_1 = a_2 = 1.0$, $a_3 = 0.3$, and $a_4 = a_5 = 0.5$. Energies are measured in the unit of hopping. (a)-(d): Evolution of the bulk nodal structure as one moves along a path in the $(\mu, \Delta)$ phase diagram of Fig. 4.1 from phase III [panels (a) and (b) with $(\mu, \Delta_s) = (-2.5, 0.5)$ and $(-2.9, 0.5)$, respectively] to phase IV [panels (c) and (d) with $(\mu, \Delta_s) = (-3.1, 0.5)$ and $(-3.1, 1.5)$, respectively]. (e) and (f): Energy spectrum in the absence of vortices for (e) the highest negative-energy state and (f) all the states with $k_y = 0$ of a $C_2$ NCS in a (100) slab geometry with the same parameters as in panel (d). (g) Energy spectrum in the presence of a vortex-antivortex pair oriented along the (110) direction as a function of momentum parallel to the vortex lines, $k_\parallel = \frac{1}{2}(k_x + k_y)$, with the same parameters as in panel (d). The subgap states are localized at the vortex cores.

winding number $\nu_1$, leads to the appearance of flat-band surface states. In addition, phase III supports $\mathbb{Z}_2$ Majorana surface states, whereas phase IV does not exhibit any additional surface states. This is exemplified in Figs. 4.4(e) and 4.4(f), which show the energy spectrum at the (100) surface of a $C_2$ NCS in phase IV. Flat-band surface states appear within regions of the surface BZ that are bounded by the projected bulk nodal rings. But otherwise there exist no additional surface states in phase IV. Indeed, the energy spectrum along the $k_z = 0$ line is fully gapped [Fig. 4.4(f)]. Using the same adiabatic deformations as before, we find that phase III can be connected to phase I, showing that the $\mathbb{Z}_2$ surface states of phase III originate from the topological properties of the fully gapped phase I. Phase IV, on the other hand, can be deformed into phase II by shrinking the nodal rings into points at opposite sides of the Fermi surface until they vanish, which corroborates our finding that there are no additional surface states in phase IV.

In contrast to NCSs with $D_4$ or $C_{4v}$ point-group symmetry, NCSs with monoclinic point-group $C_2$ do not support any zero-energy vortex-bound states, neither in the fully gapped phases I and II nor in the nodal phases III and IV. This is in line with our finding that the chiral symmetry $S$ (i.e., the combination of reflection ($\pi$ rotation), particle-hole, and time-reversal symmetry), which is present for $D_4$ and $C_{4v}$ NCSs but absent for $C_2$ NCSs, guarantees the the stability of the zero-energy vortex-bound states. The absence of zero-energy vortex states in $C_2$ point-group NCSs is
demonstrated in Fig. 4.4(g) for phase IV, which shows the energy spectrum for a vortex-antivortex pair oriented along the (110) axis, and also follows from an analytical argument, see Appendix B.1.

4.5 Summary and discussion

In summary, we have studied zero-energy vortex-bound states in 3D nodal and fully gapped NCSs. While vortex lines in NCSs with tetragonal point-group $D_4$ and $C_{4v}$ support zero-energy vortex-bound states, $C_2$ point-group NCSs do not exhibit any Majorana vortex-bound states. We have found that the existence of Majorana vortex-bound states in nodal NCSs correlates with the appearance of Majorana cone and arc surface states. The zero-energy vortex states in $C_{4v}$ ($D_4$) NCSs are protected by a combination of reflection ($\pi$ rotation), time-reversal, and particle-hole symmetry, see Eq. (4.7). This is reminiscent of the zero modes at dislocation lines of band-topological insulators which are stabilized by certain space group symmetries [113].

Our findings have implications for experiments on 3D NCSs and on heterostructures, in which topological superconductivity is induced via the proximity effect of a conventional $s$-wave superconductor [114, 115]. Vortex-bound states can be directly observed in ordinary and spin-resolved scanning tunneling microscopy [116]. The helical Majorana vortex states of $D_4$ point-group NCSs can carry currents along the vortex lines, which could in principle be detected using thermal transport measurements [107]. Moreover, the vortex-bound states are expected to be observable in terms of the cross-correlated responses between the orbital angular momentum $L$ and the thermal polarization $P_E$ of a 3D topological SC, which were recently discussed in Ref. [117]. The so-called gravitomagnetoelectric polarizability of a 3D topological SC (i.e., the analog of the magnetoelectric polarizability of a 3D topological insulator) is given by

$$\chi^{ab}_{g} = \frac{\partial L^a}{\partial E^b_g} = \frac{\partial P^g_E}{\partial \Omega^b} , \quad a, b = x, y, z,$$

(4.11)

where $\Omega$ is the (external) angular velocity of the SC and $E_g = -T^{-1}\nabla T$ represents the temperature gradient. Note that the thermal polarization $P_E$ is related to the distribution of the induced heat $Q$ via $\Delta Q = -\nabla \cdot P_E$. According to Eq. (4.11) a thermal polarization (entropy polarization) $P_E^g$ can be generated by rotating the system with angular velocity $\Omega$. The presence of vortex lines leads to an additional contribution to the angular momentum and hence to an additional accumulation of entropy (heat) at the top and bottom surfaces of the 3D SC. Vortex-bound states, on the other hand, can carry a thermal current connecting top and bottom surfaces.

\footnote{For the $C_2$ point-group NCS with $a_4 \neq 0$ and $a_5 \neq 0$, the variables $r$ and $\theta$ are not separable in the continuum BdG equation given in the Appendix B.1, which may imply that there are no zero-energy solutions localized at the vortex core.}
Chapter 5
Classification of gapless topological phases

5.1 Introduction

The topologically stable Fermi points and superconducting nodal structures in many materials as shown in previous sections can be viewed, in a sense, as momentum-space defects. This is as momentum-space analogues of real-space topological defects. In other words, the nodal points in $d_{x^2-y^2}$-wave superconductors, the Fermi points in graphene, and the nodal points in $^3$He A-phase can be interpreted as momentum-space point defects, i.e., as vortices and hedgehogs, respectively. The nodal lines in NCSs, on the other hand, correspond to momentum-space line defects, i.e., vortex lines. Similar to real-space defects, the stability of these Fermi points, nodal points, and nodal lines is guaranteed by the conservation of some topological invariant, i.e., e.g., a Chern or winding number.

In this section, building on various works [21, 38, 39, 55, 59, 118–126], we derive a classification of topologically stable Fermi surfaces in semimetals and nodal lines in superconductors using K-theory arguments [Table 5.3 in Sec. 5.2]. As it turns out, the presence of discrete symmetries, such as time-reversal symmetry (TRS) or particle-hole symmetry (PHS), plays a crucial role for the classification of gapless topological phases, a fact that has not been emphasized previously. The appearance of protected zero-energy states at the boundary of gapless topological phases is discussed, and it is shown that the existence of these boundary states is directly linked to the topological stability of the Fermi surfaces (superconducting nodal lines) in the bulk via a generalized bulk-boundary correspondence [Sec. 5.2.5]. In particular, we demonstrate that gapless topological phases in symmetry class A or AIII with stable Fermi surfaces of codimension $q > 1$ necessarily support zero-energy surface flat bands. As shown in Secs. 2 and 3, we present various examples of gapless topological phases and discuss their topological surface states.

1 By definition, a Fermi surface is a set of gapless points in the Brillouin zone. To simplify terminology, we will refer to Fermi points/lines in metals and nodal points/lines in superconductors, etc., simply as “Fermi surfaces”.

2 Hořava [118] pointed out an interesting connection between the classification of stable Fermi surfaces and the classification of stable D-branes. Making an analogy with string theory, we observe that the result by Hořava corresponds to D$p$-branes in Type IIA string theory. Hence, one might wonder what are the gapless topological objects in condensed matter physics that correspond to D$p$-branes in Type IIB string theory. Furthermore, in Type I or Type I’ string theory it is customary to consider besides D$p$-branes also orientifold hyperplanes. (Note that every space-time point on an orientifold hyperplane is identified with its mirror image.) It is known that D$p$-branes in Type I string theory are classified in terms of real K-theory [127]. Hence, one might again wonder what are the gapless topological objects in condensed matter physics that correspond to orientifold hyperplanes or D$p$-branes in Type I or Type I’ string theory. In fact, for topological insulators and superconductors, it was found that there is a one-to-one correspondence between the K-theory classification of topological insulators/superconductors and the K-theory charges of D-branes in Type IIA and Type IIB string theory, or the K-theory charges of non-BPS D-branes in Type I and I’ string theory [128][129].
5.2 Stability of Fermi surfaces

The classification of topologically stable Fermi surfaces in terms of K-theory is closely related to the classification of topologically stable zero modes localized on real space defects. In Sec. 5.2.1, we will therefore first review the stability of localized gapless modes on topological defects, before discussing the classification of topologically stable Fermi surfaces in Sec. 5.2.2. To denote the dimensionality of the Brillouin zone (BZ), the Fermi surfaces, and the real space defects we use the notation:

\[ d_{\text{BZ}} = (\text{total spatial dimension}) = (\text{total dimension of the BZ}) \]

\[ d_k = (\text{codimension of a Fermi surface}) - 1 = \left( \begin{array}{c} \# \text{ of parameters characterizing a surface} \\ \text{surrounding a Fermi surface in the BZ} \end{array} \right) \]

\[ d_r = (\text{codimension of a real space defect}) - 1 = \left( \begin{array}{c} \# \text{ of parameters characterizing a surface} \\ \text{surrounding a real space defect} \end{array} \right) \]

In other words, the dimension of a Fermi surface and a real space defect are \( d_{\text{BZ}} - d_k - 1 \) and \( d_{\text{BZ}} - d_r - 1 \), respectively.

5.2.1 Real space defects

In this subsection, we review the classification of localized gapless modes on topological defects from the K-theory point of view [55, 130]. To that end, let us consider the topology associated with gapped Hamiltonians \( H(r, k) \), where \( k = (k_1, k_2, \cdots, k_{d_{\text{BZ}}}) \) denotes the \( d_{\text{BZ}} \)-dimensional momentum coordinate, and \( r = (r_1, r_2, \cdots, r_{d_r}) \) the position-space parameters characterizing the defect. That is, \( r \) are the coordinates parametrizing the surface that encloses the defect in question. For instance, a line defect in a three-dimensional system is described by the Hamiltonian

\[ H(r, k) = k_1 \gamma_1 + k_2 \gamma_2 + k_3 \gamma_3 + m_1(x, y) \gamma_4 + m_2(x, y) \gamma_5, \]

where \( m_1(x, y) = x/\sqrt{x^2 + y^2} \), \( m_2(x, y) = y/\sqrt{x^2 + y^2} \), and \( \gamma_i \) are five \( 4 \times 4 \) anticommuting matrices. In this case, \( k_1, k_2, k_3 \in k \) and \( m_1, m_2 \in r \).

For condensed matter systems defined on a lattice, the BZ is a \( d_2 \)-dimensional torus, \( k \in T^{d_{\text{BZ}} = d_2} \), and \( r \in S^{d_r = d_1} \), where \( S^{d_1} \) is a \( d_1 \)-dimensional sphere surrounding the defect in real space. If we are interested in “strong” but not in “weak” topological insulators and superconductors, we can take \( k \in S^{d_2} \). Furthermore, it turns out it is enough to consider \((r, k) \in S^{d_1 + d_2} \) [55]. To determine the topology of the family of Hamiltonians \( H(r, k) \), one needs to examine the adiabatic evolution of the wavefunctions of \( H(r, k) \) along a closed real-space path surrounding the
complex case ($\mathbb{F} = \mathbb{C}$):

<table>
<thead>
<tr>
<th>$s$ class</th>
<th>$\delta = d_2 - d_1$</th>
<th>$\delta = d_2 - d_1$</th>
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<tr>
<td>0 A</td>
<td>$\mathbb{Z}$</td>
<td>$\mathbb{Z}$</td>
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<tr>
<td>1 AII</td>
<td>$\mathbb{Z}$</td>
<td>$\mathbb{Z}$</td>
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real case ($\mathbb{F} = \mathbb{R}$):

<table>
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<tr>
<th>$s$ class</th>
<th>$\delta = d_2 - d_1$</th>
<th>$\delta = d_2 - d_1$</th>
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<tr>
<td>0 AI</td>
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</tr>
<tr>
<td>1 BDI</td>
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<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>2 D</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>3 DIII</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>4 AII</td>
<td>$\mathbb{Z}$</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>5 CII</td>
<td>$\mathbb{Z}$</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>6 C</td>
<td>$\mathbb{Z}$</td>
<td>$\mathbb{Z}$</td>
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</tbody>
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Table 5.1: K-group $K_\mathbb{F}(s; d_1, d_2) = K_\mathbb{F}(s; \delta = d_2 - d_1)$ from Ref. [55].

defect $^3$ From this consideration, one can define a K-theory charge for $\mathcal{H}(r, k)$ and describe the stable equivalent classes of Hamiltonians $\mathcal{H}(r, k)$ in terms of the K-group

$$K_\mathbb{F}(s; d_1, d_2),$$

where $s$ represents one of the Altland-Zirnbauer (AZ) symmetry classes [122,123] given in Table 5.1. $\mathbb{F} = \mathbb{C} (\mathbb{R})$ stands for the complex (real) AZ symmetry classes, and $d_1$ and $d_2$ represent the dimensions of $r$ and $k$, respectively.

An important relation used in the analysis of Ref. [55,130] is that K-groups of different symmetry classes are related by

$$K_\mathbb{F}(s; d_1, d_2 + 1) = K_\mathbb{F}(s - 1; d_1, d_2),$$

and

$$K_\mathbb{F}(s; d_1 + 1, d_2) = K_\mathbb{F}(s + 1; d_1, d_2).$$
that the two Hamiltonians are topologically equivalent \cite{55,130}. Combining Eqs. (5.2) and (5.3), one finds

$$K_F(s; d_1 + 1, d_2 + 1) = K_F(s; d_1, d_2),$$

which shows that the topological classifications only depend on the difference

$$\delta = d_2 - d_1.$$  \hspace{1cm} (5.5)

From this, it was shown in Refs. \cite{55,130} that the classification of zero-energy modes localized on real-space topological defects is given by the K-groups $K_F(s; d_1, d_2)$ (see Table 5.1) with

$$d_1 = d_r, \quad d_2 = d_{BZ}, \quad \delta = d_{BZ} - d_r.$$ \hspace{1cm} (5.6)

In other words, whenever the K-group is nontrivial (i.e., $K_F(s; d_r, d_{BZ}) = \mathbb{Z}$ or $\mathbb{Z}_2$) the K-theory charge can take on nontrivial values, which in turn indicates the presence of one or several zero-energy modes localized on the topological defect. As a special case, the periodic table of topological insulators and superconductors \cite{6,59,125,131} is obtained from the K-groups by taking (cf. Table 5.2)

$$d_1 = 0, \quad d_2 = d_{BZ}, \quad \delta = d_{BZ}.$$ \hspace{1cm} (5.7)

Representative Hamiltonians of the stable equivalent classes of $\mathcal{H}(r, k)$ can be constructed in terms of linear combinations of anticommuting Dirac matrices \cite{55} (see also \cite{6}). For instance, consider

$$\mathcal{H}(r, k) = R^\mu(r, k)\gamma_\mu + K^i(r, k)\gamma_i,$$ \hspace{1cm} (5.8)

with “position-type” Dirac matrices $\gamma_\mu$ and “momentum-type” Dirac matrices $\gamma_i$, where $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$, $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$, and $\{\gamma_\mu, \gamma_i\} = 0$. If the Hamiltonian satisfies time-reversal symmetry $T$, we require

$$[\gamma_\mu, T] = \{\gamma_i, T\} = 0,$$ \hspace{1cm} (5.9)

while for particle-hole symmetry $P$, we have

$$\{\gamma_\mu, P\} = [\gamma_i, P] = 0.$$ \hspace{1cm} (5.10)
<table>
<thead>
<tr>
<th></th>
<th>$d_1$</th>
<th>$d_2$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>insulators (fully gapped SCs)</td>
<td>0</td>
<td>$d_{\text{BZ}}$</td>
<td>$d_{\text{BZ}}$</td>
</tr>
<tr>
<td>zero modes localized on real-space defects in insulators (fully gapped SCs)</td>
<td>$d_r$</td>
<td>$d_{\text{BZ}}$</td>
<td>$d_{\text{BZ}} - d_r$</td>
</tr>
<tr>
<td>Fermi surfaces at high-symmetry points</td>
<td>0</td>
<td>$d_k$</td>
<td>$d_k + 2$</td>
</tr>
</tbody>
</table>

Table 5.2: Assignment of dimensions ($d_1$, $d_2$) for different classification schemes: (i) classification of insulators (fully gapped superconductors), (ii) classification of zero modes localized on real-space defects in insulators (fully gapped superconductors), and (iii) classification of Fermi surfaces.

Under the antiunitary symmetries $T$ and $P$ the coefficients $R^\mu(r,k)$ and $K^i(r,k)$ transform in the same way as position and momentum, respectively, i.e., $R^\mu(r,-k) = R^\mu(r,k)$ and $K^i(r,-k) = -K^i(r,k)$. As shown in Ref. [55], a representative Hamiltonian of the real symmetry class $s$ can be constructed in terms of a linear combination of $b+1$ position-type matrices $\gamma_\mu$ and $a$ momentum-type matrices $\gamma_i$, with $a - b = s \mod 8$.

### 5.2.2 Fermi surfaces (momentum-space defects)

The analysis of Refs. [55, 130], which we have reviewed above, can be extended to study the topological stability of Fermi surfaces. For a given Hamiltonian $\mathcal{H}(k)$, we define the Fermi surface as the momentum-space manifold where $\mathcal{H}(k) = 0$\(^4\). The key observation is that topologically stable Fermi surfaces can be viewed as defects in the momentum-space structure of the wavefunctions of $\mathcal{H}(k)$. Hence, in order to determine the topology of a $(q = d_{\text{BZ}} - d_k - 1)$-dimensional Fermi surface, we need to examine the adiabatic evolution of the wavefunctions of $\mathcal{H}(k)$ along a closed momentum-space path surrounding the Fermi surface. This closed path in momentum space is parametrized by $d_k$ variables, i.e., it defines a $d_k$-dimensional hypersphere $S^{d_k} = S^{d_{\text{BZ}} - q - 1} \subset S^{d_{\text{BZ}}} = \text{BZ}$ surrounding the Fermi surface. As mentioned in Refs. [111, 132], the symmetry transformation (TRS or/and PHS) of this $d_k$-dimensional hypersphere is not simple as $k \rightarrow -k$. In order to resolve this issue, we need to introduce a dimension-raising map that maps a Hamiltonian $\mathcal{H}(\kappa)$ on $S^{d_k}$ into $\mathcal{H}(\kappa, \kappa_{d_k+1})$ on $S^{d_k+1}$ isomorphically [see Ref.[111] and App. C.1]. Then, we can classify a $q$-dimensional Fermi surface in $d_{\text{BZ}}$ dimensions from the mapped Hamiltonian $\mathcal{H}(\kappa, \kappa_{d_k+1})$ by using K-theory directly.

The dimension-raising map can be constructed in two different ways based on the presence or absence of chiral symmetry in the original Hamiltonian $\mathcal{H}(\kappa)$

$$\mathcal{H}_{nc}(\kappa, \kappa_{d_k+1}) = \sin \kappa_{d_k+1} \mathcal{H}_c(\kappa) + \cos \kappa_{d_k+1} \mathcal{S}, \quad \kappa_{d_k+1} \in [0, \pi],$$

$$\mathcal{H}_c(\kappa, \kappa_{d_k+1}) = \sin \kappa_{d_k+1} \mathcal{H}_{nc}(\kappa) \otimes \tau_z + \cos \kappa_{d_k+1} \mathcal{I} \otimes \tau_\alpha, \quad \kappa_{d_k+1} \in [0, \pi],$$

\(^4\)Alternatively, the Fermi surface can be defined in terms of the poles of the single particle Green’s function.
where $H_c(H_{nc})$ denotes the presence (absence) of chiral symmetry in the Hamiltonian, $S$ is the chiral symmetry operator for the original Hamiltonian $H_c(\kappa)$, and $\alpha = x$ (or $y$) depends on the original Hamiltonian $H_{nc}(\kappa)$ with TRS (or PHS)\(^5\).

The mapped Hamiltonian $H(\kappa, \kappa_{d+1})$ is on a $(d_k + 1)$-dimensional sphere, which can be represented as $k_1^2 + k_2^2 + \cdots + k_{d+1}^2 + k_{d+2}^2 = r^2$. Notice that TRS and/or PHS transform $(k_1, k_2, \cdots, k_d, k_{d+1}) \to (-k_1, -k_2, \cdots, -k_d, k_{d+1})$.

We can parametrize $\kappa_i$ with the following form

$$\kappa_i = \frac{k_i}{r + k_{d+2}}, \quad i = 1, \cdots, d_k + 1. \tag{5.13}$$

Then TRS and/or PHS transform $(\kappa, \kappa_{d+1}) \to (-\kappa, -\kappa_{d+1})$. The mapped Hamiltonian satisfies

$$T^\dagger H(\kappa, \kappa_{d+1}) T = H(-\kappa, -\kappa_{d+1}),$$
$$P^\dagger H(\kappa, \kappa_{d+1}) P = -H(-\kappa, -\kappa_{d+1}). \tag{5.14}$$

For the complex case $F = \mathbb{C}$ in AZ symmetry classes, Eqs. (5.11) and (5.12) show that the classification of a $q$-dimensional Fermi surface is equivalent to the classification of the mapped Hamiltonian, which is in $(d_k + 1)$ dimensions with a shift of symmetry classes of the original Hamiltonian by one.

For the real case $F = \mathbb{R}$ in AZ symmetry classes, the mapped Hamiltonian $H_{nc}(\kappa, \kappa_{d+1})$ in Eq. (5.11) breaks TRS or PHS due to the second term. Since chiral symmetry $S = T^\dagger P$, we have $T^\dagger S T = \eta_T T S$ and $P^\dagger S P = \eta_P S$, where $\eta_T (\eta_P)$ is the sign of the TRS (PHS) in Table 5.3. The mapped Hamiltonian breaks TRS if $\eta_T = -1$ and breaks PHS if $\eta_P = +1$. On the other hand, for $F = \mathbb{R}$ in AZ symmetry classes, the mapped Hamiltonian $H_c(\kappa, \kappa_{d+1})$ in Eq. (5.12) has an additional PHS (TRS) with $T \otimes \tau_y (P \otimes \tau_x)$ when the original Hamiltonian $H_{nc}(\kappa)$ has TRS (PHS).

As a result, the original Hamiltonian in $d_k$ dimensions with symmetry class $s$ maps to the mapped Hamiltonian in $(d_k + 1)$ dimensions with symmetry class $(s - 1)$. Hence the K-theory charge of a $q$-dimensional Fermi surface in $d_{BZ}$ dimensions with $s$ symmetry class is given by K-group

$$K_{FS}^q(s, d_1, d_2) = K_F(s - 1; d_1, d_2 + 1) = K_F(s; d_1, d_2 + 2) = K_F(s; \delta), \tag{5.15}$$

with

$$d_1 = 0, \quad d_2 = d_k, \quad \delta = d_k + 2, \tag{5.16}$$

\(^5\)Here we consider real AZ symmetry classes. For complex AZ symmetry classes, the chiral symmetry for Eq. (5.12) is $S = 1 \otimes \tau_x \tau_x$.
complex case ($d_{\text{BZ}} = 2$):

<table>
<thead>
<tr>
<th>class</th>
<th>$T$</th>
<th>$P$</th>
<th>$S$</th>
<th>$d_k = 0$</th>
<th>$d_k = 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
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<td>0</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
</tr>
<tr>
<td>ALL</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
</tr>
</tbody>
</table>

complex case ($d_{\text{BZ}} = 3$):

<table>
<thead>
<tr>
<th>class</th>
<th>$d_k = 0$</th>
<th>$d_k = 1$</th>
<th>$d_k = 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>ALL</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
</tr>
</tbody>
</table>

real case ($d_{\text{BZ}} = 2$):

<table>
<thead>
<tr>
<th>class</th>
<th>$T$</th>
<th>$P$</th>
<th>$S$</th>
<th>$d_k = 0$</th>
<th>$d_k = 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AI</td>
<td>+1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>BDI</td>
<td>+1</td>
<td>+1</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>D</td>
<td>0</td>
<td>+1</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
</tr>
<tr>
<td>DIII</td>
<td>−1</td>
<td>+1</td>
<td>1</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>ALL</td>
<td>−1</td>
<td>0</td>
<td>0</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>CII</td>
<td>−1</td>
<td>−1</td>
<td>1</td>
<td>0</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>C</td>
<td>0</td>
<td>−1</td>
<td>0</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>CI</td>
<td>+1</td>
<td>−1</td>
<td>1</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
</tr>
</tbody>
</table>

real case ($d_{\text{BZ}} = 3$):

<table>
<thead>
<tr>
<th>class</th>
<th>$d_k = 0$</th>
<th>$d_k = 1$</th>
<th>$d_k = 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>AI</td>
<td>0</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>BDI</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>D</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>DIII</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
</tr>
<tr>
<td>ALL</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}$</td>
</tr>
<tr>
<td>CII</td>
<td>0</td>
<td>$\mathbb{Z}_2$</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>C</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
<td>$\mathbb{Z}_2$</td>
</tr>
<tr>
<td>CI</td>
<td>0</td>
<td>$\mathbb{Z}$</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 5.3: Classification of topologically stable Fermi surfaces in two- and three-dimensional systems ($d_{\text{BZ}} = 2$ and $d_{\text{BZ}} = 3$, respectively) as a function of Fermi-surface dimension $q = d_{\text{BZ}} - d_k - 1$ and symmetry class of $\mathcal{H}(k)$ restricted to a hypersphere $S^{d_k}$ surrounding an individual Fermi surface. Ten symmetry classes are distinguished, depending on the presence or absence of time-reversal symmetry ($T$), particle-hole symmetry ($P$), and chiral (or sublattice) symmetry ($S$). The labels $T$, $P$, and $S$ indicate the presence or absence of time-reversal, particle-hole, and chiral symmetries, respectively, as well as the types of these symmetries.

i.e., by $K_p(s; \delta = d_k + 2)$, where $d_k = d_{\text{BZ}} - q - 1$. That is, the classification (or “periodic table”) of topologically stable Fermi surfaces in symmetry class $s$ can be inferred from Table 5.1 together with Table 5.2. For two- and three-dimensional systems, the classification of $q$-dimensional Fermi surfaces is explicitly given in Table 5.3.

Let us construct a few simple examples of topologically stable (and unstable) Fermi surfaces in terms of Dirac Hamiltonians defined in the continuum. Examples of topological Fermi surfaces defined in terms of lattice Hamiltonians will be discussed in Sec. 3.1.

Class A. We first consider single-particle Hamiltonians $\mathcal{H}(k)$ with Fermi surfaces in symmetry class A, i.e., Fermi surfaces that are not invariant under time-reversal, particle-hole, and chiral symmetry. Below we list examples of

---

6Focusing on noninteracting systems, we study the topological stability of Fermi surfaces in terms of Bloch or Bogoliubov-de Gennes Hamiltonians. However, it is straightforward to extend our analysis to the Green’s function formalism describing weakly (or moderately weakly) interacting systems (see Refs. [55, 138, 133] and compare with Ref. [134]).
Hamiltonians in $d_{BZ}$ spatial dimensions with Fermi surfaces in symmetry class A

<table>
<thead>
<tr>
<th>Hamiltonian</th>
<th>Fermi surface dimension $q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{H}(k) = k_1$</td>
<td>$d_{BZ} - 1$</td>
</tr>
<tr>
<td>$\mathcal{H}(k) = k_1\sigma_1 + k_2\sigma_2$</td>
<td>$d_{BZ} - 2$</td>
</tr>
<tr>
<td>$\mathcal{H}(k) = k_1\sigma_1 + k_2\sigma_2 + k_3\sigma_3$</td>
<td>$d_{BZ} - 3$</td>
</tr>
<tr>
<td>$\mathcal{H}(k) = k_1\alpha_1 + k_2\alpha_2 + k_3\alpha_3 + k_4\beta$</td>
<td>$d_{BZ} - 4$</td>
</tr>
<tr>
<td>:</td>
<td>:</td>
</tr>
</tbody>
</table>

(5.17)

Here, $\sigma_{1,2,3}$ denote the three Pauli matrices, while $\alpha_{1,2,3}$ and $\beta$ represent the four Dirac matrices (gamma matrices). For each example, the Fermi surface is given by the manifold \{ $k$; with $k_i = 0$ for $i = 1, 2, \cdots, d_{BZ} - q$ \}, where $q$ is the dimension of the Fermi surface. In the above examples, Fermi surfaces with $d_{BZ} - q$ odd (i.e., $d_k + 1$ odd) are perturbatively stable against any deformation of the Hamiltonian. Fermi surfaces with $d_{BZ} - q$ even, on the other hand, are topologically unstable (see Hořava [118]). Due to the absence of a spectral symmetry (i.e., no chiral symmetry) in class A, we can add a nonzero chemical potential term $\mu I$ to the Hamiltonians in Eq. (5.17). Thus, for example, the $(d_{BZ} - 3)$-dimensional stable Fermi surface of $\mathcal{H}(k) = k_1\sigma_1 + k_2\sigma_2 + k_3\sigma_3$ can be turned into a stable Fermi surface of dimension $d_{BZ} - 1$ upon inclusion of a finite chemical potential. Note that the third row in the above list, i.e., $\mathcal{H}(k) = k_1\sigma_1 + k_2\sigma_2 + k_3\sigma_3$, corresponds to a Weyl semimetal [23–36].

Class AIII. Second, we consider Hamiltonians with Fermi surfaces in symmetry class AIII. Recall that due to the presence of chiral symmetry in class AIII (i.e., \{ $\mathcal{H}(k), U_S$ \} = 0, where $U_S$ is an arbitrary unitary matrix), the chemical potential is pinned at $\mu = 0$. Below we list a few examples of topologically stable (and unstable) Fermi surfaces in symmetry class AIII

<table>
<thead>
<tr>
<th>Hamiltonian</th>
<th>Fermi surface dimension $q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{H}(k) = k_1\sigma_1$</td>
<td>$d_{BZ} - 1$</td>
</tr>
<tr>
<td>$\mathcal{H}(k) = k_1\sigma_1 + k_2\sigma_2$</td>
<td>$d_{BZ} - 2$</td>
</tr>
<tr>
<td>$\mathcal{H}(k) = k_1\alpha_1 + k_2\alpha_2 + k_3\alpha_3$</td>
<td>$d_{BZ} - 3$</td>
</tr>
<tr>
<td>$\mathcal{H}(k) = k_1\alpha_1 + k_2\alpha_2 + k_3\alpha_3 + k_4\beta$</td>
<td>$d_{BZ} - 4$</td>
</tr>
<tr>
<td>:</td>
<td>:</td>
</tr>
</tbody>
</table>

(5.18)

Here, we find that Fermi surfaces with dimension $d_{BZ} - q$ even are topologically stable, whereas those with $d_{BZ} - q$ odd are topologically unstable.
In passing, we remark that the above analysis can also be applied to gapless Hamiltonians defined in an extended parameter space, i.e., Hamiltonians that are parametrized by momentum coordinates and some external control parameters, such as, e.g., mass terms $m_i$. The topological arguments can then be used to predict the existence of extended regions of gapless phases in the topological phase diagram (see, e.g., Refs. [23, 60, 135]).

5.2.3 Comments on the stability of multiple Fermi surfaces

It should be stressed that the above topological stability criterion (i.e., Table 5.3) applies only to individual Fermi surfaces. That is, in the above analysis we considered the wavefunction evolution along a hypersphere $S^d_k$ that encloses a single Fermi surface located at high symmetric points in the BZ. However, many lattice Hamiltonians exhibit multiple Fermi surfaces that are located in different regions of the BZ. In that situation, one can either consider the wavefunction evolution along hyperspheres $S^d_k$ that surround more than one Fermi surface, or study the topological stability of each Fermi surface separately. Depending on this choice of $S^d_k$ one generally finds different stability characteristics. In the following, we make a few remarks on the topological stability of these multiple Fermi surfaces.

Fermion doubling. Due to the Fermion doubling theorem [136], certain topologically stable Fermi surfaces, which in the continuum limit are described in terms of Dirac Hamiltonians, (e.g., the Weyl semi-metal) cannot be realized as single Fermi surfaces in lattice systems. That is, on a lattice these Fermi surfaces always appear in pairs with opposite K-theory charges. In that case the Fermi surfaces are not protected against commensurate perturbations, such as charge-density-wave, spin-density-wave, or other nesting-type perturbations that connect Fermi surfaces with opposite K-theory charges. However, these Fermi surfaces are individually stable, i.e., stable against deformations that do not lead to nesting instabilities.

Effective symmetry classes. In the presence of multiple Fermi surfaces, anti-unitary symmetries (i.e., TRS and PHS) can act in two different ways on the system: (i) the symmetry maps different Fermi surfaces onto each other, or (ii) each individual Fermi surface is (as a set) invariant under the symmetry transformation. In case (i) the symmetry class of the entire system is distinct from the symmetry class of each individual Fermi surface. Hence, the topological number describing the stability of an individual Fermi surface differs from the topological invariant characterizing the entire system.

Fermion surfaces off high-symmetry points When the Fermi surfaces are located away from high symmetry points of the BZ, the hyperspheres $S^d_k$ encircling the Fermi surfaces do not have the proper momentum transformation under TRS and/or PHS. Hence K-theory is not applicable to classify the stability of Fermi surfaces. Nevertheless, a classification table of Fermi surfaces off high-symmetry points is given in Ref. [137]. The resulting classification
Table 5.4: Classification of topologically stable Fermi surfaces located off high-symmetric points of the BZ in two- and three-dimensional systems ($d_{BZ} = 2$ and $d_{BZ} = 3$, respectively) as a function of Fermi-surface dimension $q = d_{BZ} - d_k - 1$ and symmetry class of $\mathcal{H}(k)$ restricted to a hypersphere $S^{d_k}$ surrounding an individual Fermi surface. Ten symmetry classes are distinguished, depending on the presence or absence of time-reversal symmetry ($T$), particle-hole symmetry ($P$), and chiral (or sublattice) symmetry ($S$). The labels $T$, $P$, and $S$ indicate the presence or absence of time-reversal, particle-hole, and chiral symmetries, respectively, as well as the types of these symmetries.

table is shown in Table 5.4, which can also be obtained by replacing $\delta = d_k + 2 \to \delta = d_k$ in Eq. 5.15

5.2.4 Classification of gapless topological phases from higher dimensional topological insulators and superconductors.

Here we derive an alternative classification of gapless topological phases in terms of symmetries of the entire system (as opposed to the symmetries of $\mathcal{H}(k)$ restricted to a hypersphere $S^{d_k}$ surrounding an individual Fermi surface as in Sec. 5.2.2). To that end, we apply a dimensional reduction procedure to obtain $d_{BZ}$-dimensional gapless topological phases from the zero-energy boundary modes of $(d_{BZ} + 1)$-dimensional topological insulators (fully gapped superconductors). Namely, we observe that the surface states of $(d_{BZ} + 1)$-dimensional topological insulators can be interpreted as topologically stable Fermi surfaces in $d_{BZ}$ dimensions. In fact, as was shown in Ref. [138], the bulk topological invariant of a $(d_{BZ} + 1)$-dimensional topological insulator is directly related to the K-theory topological charge of the boundary Fermi surface. Hence, we argue that the two Fermi surfaces that appear on either side of a $(d_{BZ} + 1)$-dimensional topological insulator can be embedded in a $d_{BZ}$-dimensional BZ. Moreover, we recall from Sec. 5.2.2 that the classification of stable Fermi surfaces only depends on the codimension ($d_k + 1$) of the Fermi sur-
face, since a \( q \)-dimensional stable Fermi surface in \( d_{\text{BZ}} \) dimensions can always be converted into a \((q+1)\)-dimensional stable Fermi surface in \( d_{\text{BZ}} + 1 \) dimensions by including an extra momentum-space coordinate. Based on these arguments we find that the classification of \((q = d_{\text{BZ}} - d_k - 1)\)-dimensional Fermi surfaces in terms of symmetries of the total system is obtained from Table 5.1 with \( \delta = d_k + 2 \), which is identical to the classification by using K-theory arguments (see Table 5.3).

Note that in the above construction of gapless topological phases the stable Fermi surfaces always appear in pairs (one from each of the two surfaces of the topological insulator) due to the Fermion doubling theorem. Therefore, these gapless topological phases are unstable against commensurate nesting-type deformations that connect Fermi surfaces with opposite K-theory charges.

5.2.5 Bulk-boundary correspondence

Topological characteristics of stable Fermi surfaces can lead to the appearance of zero-energy surface states via a bulk-boundary correspondence. We discuss this phenomenon in terms of a few specific examples defined in the continuum (similar considerations are applied to lattice systems in Secs. 2 and 3).

Fermi rings in three-dimensional systems. Consider first the case of two topologically stable Fermi rings in a three-dimensional system described by the Hamiltonian \( \mathcal{H}(k) \) (see Fig. 5.1). These rings of gapless points occur, for example, in nodal topological superconductors (e.g., class DIII, AIII, or CI, see Sec. 3.1), or in topological semi-metals with sublattice symmetry (class AIII) [139]. The topological characteristics of these Fermi rings is determined by the topology of the wavefunctions along a circle \( S^d_k = 1 \) enclosing the Fermi ring (red circle in Fig. 5.1(c)). That is, the stability of the Fermi ring is guaranteed by the conservation of a topological charge, which is given in terms of the homotopy number of the map of \( S^d_k = 1 \) onto the space of Hamiltonians.

Let us now discuss the appearance of zero-energy states at a two-dimensional surface of this system. To that end, we define a two-dimensional surface BZ (gray planes in Fig. 5.1) parametrized by the two surface momenta \( k_{1,||} \) and \( k_{2,||} \). The third momentum component, which is perpendicular to the surface BZ, is denoted by \( k_{\perp} \). The appearance of a zero-energy state at a given surface momentum \( k_{||}^0 = (k_{1,||}^0, k_{2,||}^0) \) can be understood by considering a continuous deformation of the closed path \( S^1 \) in Fig. 5.1(c) into a infinite semi-circle (Fig. 5.1(a)), such that the diameter of the semi-circle is parallel to \( k_{\perp} \) and passes through \( k_{||}^0 = (k_{1,||}^0, k_{2,||}^0) \). This path deformation does not alter the value of the topological number (i.e., the K-theory topological charge), as long as no Fermi ring is crossed during the deformation process. Furthermore, one can show that in the limit of an infinitely large semi-circle, the topological charge of the Fermi ring is identical to the topological number of the one-dimensional system \( \mathcal{H}(k_{\perp}, k_{||}^0) \). Hence, there appear zero-energy surface states at those momenta \( k_{||}^0 \), where the corresponding one-dimensional gapped Hamiltonian \( \mathcal{H}(k_{\perp}, k_{||}^0) \)
Figure 5.1: Illustration of integration path deformation in the three-dimensional BZ. The gray planes represent the two-dimensional surface BZ parametrized by the two surface momenta $k_{1,\parallel}$ and $k_{2,\parallel}$. The light and dark blue areas indicate regions in the surface BZ where there appear zero-energy states.

<table>
<thead>
<tr>
<th>dimension of BZ ($d_{BZ}$)</th>
<th>dimension of FS ($q$)</th>
<th>dim. of sphere surrounding FS ($d_k$)</th>
<th>dimension of surface flat band</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
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<tr>
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</tr>
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</tr>
<tr>
<td>4</td>
<td>2</td>
<td>1</td>
<td>3</td>
</tr>
</tbody>
</table>

Table 5.5: Dimensionality of zero-energy flat bands appearing at the boundary of a $d_{BZ}$-dimensional system with a $q$-dimensional stable Fermi surface in symmetry class A or AIII.

has a nontrivial topological characteristics, i.e., at momenta that lie inside the projections of the Fermi rings of the bulk system. For the complex symmetry classes (i.e., class AIII for the present case) it follows that the zero-energy surface states occur in two-dimensional regions in the surface BZ that are bounded by the projections of the Fermi rings [light and dark blue areas in Fig. 5.1.40,42]. In other words, the zero-energy states form two-dimensional surface flat bands. For the real symmetry classes (i.e., for symmetries that relate $+k$ to $-k$ in momentum space), it follows that zero-energy states appear at certain symmetry-invariant surface momenta that lie inside the projections of the Fermi rings [40,42].

**Fermi points in three-dimensional systems.** As a second example, let us consider a three-dimensional system $\mathcal{H}(k)$ with two topologically stable Fermi points. Topologically stable Fermi points can be found, for example, in Weyl semimetals (class A) [23,30,32,36]. The stability of these Fermi points is ensured by the conservation of the homotopy number of the map of $S^{d_k=2}$ onto the space of Hamiltonians, where $S^{d_k=2}$ surrounds one of the two Fermi points. To derive the existence of surface states on a given line, say, $\mathcal{L}(k_{2,\parallel}^0) = \{(k_{1,\parallel}, k_{2,\parallel}^0); \text{ with } k_{1,\parallel} \in \mathbb{R} \text{ and } k_{2,\parallel}^0 \text{ fixed}\}$.
within the surface BZ, we consider a continuous deformation of the sphere $S^2$ into a half-sphere, such that the diameter of the half-sphere is perpendicular to the surface BZ and passes through $L(k_0^0, \|)$. As before, one can show that in the limit of an infinitely large half-sphere, the topological charge of the Fermi point enclosed by the half-sphere is identical to the topological invariant of the two-dimensional system $\mathcal{H}(k_\perp, k_1, \|; k_0^0)$. Thus, there appears a linearly dispersing surface state within $L(k_0^0, \|)$, whenever the fully gapped two-dimensional Hamiltonian $\mathcal{H}(k_\perp, k_1, \|; k_0^0)$ has a nontrivial topological character. For symmetry class A, we can repeat this argument for arbitrary $k_0^0$. Therefore there exists a line of zero-energy modes in the surface BZ (i.e., an arc surface state) connecting the two projected Fermi points.

It is straightforward to generalize the above considerations to Fermi surfaces with arbitrary codimensions, provided that $d_k > 1$. The result is summarized in Table 5.5. We find that for a $q$-dimensional topologically stable Fermi surface in symmetry classes A or AIII, there appears a $(q+1)$-dimensional zero-energy flat band at the boundary of the system. For $d_k = 0$, however, which corresponds to stable Fermi surfaces of codimension 1 (i.e., e.g., a two-dimensional Fermi surface in a three-dimensional BZ), there is no topological state appearing at the boundary of the system. The reason for this is that a Fermi surface of codimension 1 cannot be surrounded by a hypersphere in momentum space, since the Fermi surface separates the BZ into two distinct regions.

### 5.3 Summary and discussion

In this section, we developed a general and unified classification of topologically stable Fermi surfaces in semimetals and superconducting nodes in superconductors in terms of discrete symmetries and spatial dimension. Using K-theory arguments, we have shown that stable Fermi surfaces can be classified in a similar manner as fully gapped topological states [see Table 5.3]. Many further developments of classifying topological gapless systems are discussed in Refs [111, 132, 137, 140]. The remarkable topological properties of these stable Fermi surfaces and superconducting nodes manifest themselves in the appearance of protected zero-energy states at the boundary of the system. In fact, the presence of topological boundary modes is directly linked to the topological structure of the bulk wavefunctions via a bulk-boundary correspondence. Depending on the case, these topological surface states form either one- or two-dimensional flat bands, or linearly dispersing Dirac or Majorana states (see Sec. 5.2.5). It should be possible to detect these different surface states using various experimental probes, such as angle-resolved photoemission measurements, scanning tunneling spectroscopy, or angle-resolved thermal transport measurements [141].

To illustrate the general principles of the classification scheme, we have examined a few concrete examples, specifically of stable nodal lines in three-dimensional NCSs [Sec. 3]. These nodal superconductors exhibit dispersionless zero-energy surface states (i.e., surface flat bands) of topological origin. An important experimental fingerprint of
these zero-energy flat bands is a zero-bias peak in the surface density of states, which depends strongly on the surface orientation. This dependence can be used as a probe of the pairing symmetry and the bulk nodal structure of the superconductor. We have also studied the stability of the surface flat bands against disorder and time-reversal symmetry breaking perturbations.

For some of the gapless topological states listed in Table 5.3 physical realizations are known and their surface states have been studied extensively. E.g., zero-energy boundary modes have been experimentally observed in graphene [12–14] and in $d_{x^2-y^2}$-wave high-temperature superconductors [18–20]. For other entries in Table 5.3 candidate materials have been proposed, but the topological surface state have not yet been conclusively observed. This includes nodal noncentrosymmetric superconductors (class DIII or AIII, $d_k = 1$), with the candidate materials CePt$_3$Si [78], Li$_2$Pt$_3$B [74], and BiPd [77], and Weyl semi-metals (class A, $d_k = 2$), which might be realized in Y$_2$Ir$_2$O$_7$ [24,27] or in HgCr$_2$Se$_4$ [25]. Finally, there are also other entries in Table 5.3 for which no physical realization is as yet known. We hope that our results will spur further experimental investigates of these interesting gapless topological states.
Chapter 6

Symmetry-protected entangling boundary zero modes in crystalline topological insulators

6.1 Introduction

One of the fundamental distinctive feature of phases of matter is the spontaneous breaking of symmetries. As a corollary, phases of matter are gapless under very general conditions when the broken symmetry group is continuous. There are, however, incompressible phases of matter at zero temperature that are featureless from the point of view of spontaneous symmetry breaking. Examples thereof are the integer quantum Hall effect (IQHE) and topological insulators (superconductors). Such incompressible phases of matter are inherently quantum mechanical. They have no classical counterparts, unlike phases breaking spontaneously a symmetry. They are characterized by topological attributes such as a quantized response function or the existence of (symmetry protected) gapless modes that propagate along a physical boundary, while they are exponentially localized away from the physical boundary (in short gapless boundary modes or edge states), when the ground state is non-degenerate in the thermodynamic limit. Another probe of their topological character is the entanglement of their incompressible ground state, whether short ranged when the ground state is non-degenerate (as in the IQHE), or long ranged when the ground states becomes degenerate in the thermodynamic limit [as in the fractional quantum Hall effect (FQHE)].

One probe that measures the entanglement of an incompressible ground state $|\Psi\rangle$ is the entanglement entropy (von Neumann entropy) defined by

$$S_A := -\text{tr}_A \left( \hat{\rho}_A \ln \hat{\rho}_A \right).$$  \hspace{1cm} (6.1a)

Here, the total system is divided into two subsystems $A$ and $B$,

$$\hat{\rho}_A := \text{tr}_B |\Psi\rangle \langle \Psi|$$  \hspace{1cm} (6.1b)

is the reduced density matrix obtained by tracing over the states in subsystem $B$ of the total density matrix

$$\hat{\rho} := |\Psi\rangle \langle \Psi|$$  \hspace{1cm} (6.1c)
in the incompressible ground state $|\Psi\rangle$. In this chapter, we will almost exclusively consider single-particle Hamiltonians, their non-degenerate incompressible ground states $|\Psi\rangle$, and partitionings into $A$ and $B$ with respect to a referred basis for which locality is manifest. We will also assume that it is possible to associate with $A$ and $B$ two regions of $d$-dimensional position space sharing a $(d-1)$-dimensional boundary. This boundary is called the entangling boundary of the partition into $A$ and $B$. This entangling boundary is unrelated to any physical boundary selected by the choice of open boundary conditions.

Another probe for the entanglement contained in an incompressible ground state $|\Psi\rangle$ is the entanglement spectrum. On the one hand, topological phases that are characterized by the presence of gapless boundary states in the energy spectrum must support gapless modes that propagate along the entangling boundary but decay exponentially fast away from the entangling boundary (in short entangling boundary states or entangling edge modes) in the entanglement spectrum. On the other hand, there are symmetry-protected topological phases that do not show gapless boundary modes in the energy spectrum, while they do show gapless boundary modes in the entanglement spectrum. The entanglement spectrum can thus be thought of as a more refined diagnostic for identifying and classifying topological incompressible ground states than the energy spectrum. For example, non-interacting insulators that owe their topological character to the existence of an inversion symmetry, may support mid-gap states in the entanglement spectrum that are protected by the inversion symmetry, while they need not support gapless boundary modes in the energy spectrum. These mid-gap modes in the entanglement spectrum cannot be removed by an adiabatic and local deformation of the single-particle Hamiltonian. As such there existence may be used as a mean to quantify a topological invariant. Symmetry protected topological phases can also arise from other discrete symmetries, such as reflection symmetry, or more general point-group symmetries. Moreover, it is known that the eigenvalues of discrete symmetry operators at the symmetric points in the Brillouin zone (BZ) are related to the number of the mid-gap states in the entanglement spectrum for inversion- and point-group-symmetric topological ground states.

In this chapter, we explain how crystalline symmetries of single-particle Hamiltonians with an incompressible ground state manifest themselves in the entanglement spectrum and how they can protect gapless boundary states in the entanglement spectrum, when no such protection is operative for the boundary states in the energy spectrum due to the non-local character of crystalline symmetries.

This chapter is organized as follows. In Sec. 6.2 after some preliminary definitions in Secs. 6.2.1 and 6.2.1 we show that the entanglement Hamiltonian is an example of supersymmetric quantum mechanics in Sec. 6.2.1. The main result of this chapter follows in Sec. 6.2.1 where we show under what conditions a crystalline symmetry can induce a spectral symmetry of the entanglement spectrum that is absent from the energy spectrum of a single-particle Hamiltonian with an incompressible ground state. The subtle interplay between the geometry imposed
by the boundary conditions, the non-local crystalline symmetry, and its (local) realization on the physical (entangling) boundaries is explained in Sec. 6.3. We then apply our main result, Eqs. (6.46) and (6.53), to the stability analysis of gapless edge states in the energy and entanglement spectra for four examples of single-particle Hamiltonians with incompressible ground states in Secs. 6.4, 6.5, 6.6, and 6.7 respectively. This stability analysis is the most intricate when treating a one-dimensional tight-binding model with inversion symmetry in Sec. 6.4. Two copies of a pair of Chern insulators differing by the sign of their Chern numbers that accommodate a reflection symmetry are treated in Sec. 6.5 as the first two-dimensional example. By considering two copies of the filled lowest Landau level with opposite Chern numbers, we treat the example of two reflection symmetries in two dimensions in Sec. 6.6. We close the applications of Eqs. (6.46) and (6.53) by demonstrating that the Kekule distortion of graphene (see Ref. [172]) should be thought of as a crystalline topological insulator. We conclude in Sec. 6.8.

### 6.2 Symmetries and entanglement spectrum

The goal of this section is to study the relationship between the symmetries shared by a fermionic Hamiltonian and its ground state and the symmetries of the reduced density matrix of the pure-state density matrix constructed from the ground state, whereby the reduced density matrix presumes a partitioning of the fermionic Fock space into the tensor product of two Fock subspaces, i.e., the decomposition of the single-particle Hilbert space into the direct sum of two subspaces.

We shall begin by studying the non-interacting case in Sec. 6.2.1. The non-interacting limit is defined in Sec. 6.2.1. The ground state for $N_f$ fermions hopping between the sites and orbitals of a lattice is a Slater determinant (Fermi sea). By Wick’s theorem, all the information contained in the density matrix for the Fermi sea can be retrieved from the equal-time one-point correlation function (matrix) and conversely, as is reviewed in Sec. 6.2.1. The direct sum decomposition of the single-particle Hilbert space is an example of a graded vector space. We show in Sec. 6.2.1 that this grading allows to construct from the equal-time one-point correlation matrix a supersymmetric single-particle Hamiltonian. This supersymmetry has consequences for the spectral properties of the reduced density matrix (entanglement spectrum) as is shown in Sec. 6.2.1 where we demonstrate that certain symmetries of the Hamiltonian induce symmetries of the entanglement spectrum. Conversely, we show in Sec. 6.2.1 that a spectral symmetry of the Hamiltonian can turn into a symmetry of the reduced density matrix in view of the hidden supersymmetry of the latter. Spectral symmetry of the Hamiltonian can thus turn into degeneracies of the entanglement spectrum.

The interacting case is considered in Sec. 6.2.2. We show how a symmetry of the Hamiltonian and of its ground state that interchanges the partition is realized on the reduced density matrix.
6.2.1 Non-interacting fermions

Hamiltonian

We consider a lattice \( \Lambda \subset \mathbb{Z}^d \) whose \( N \) sites are labeled by the vector \( \mathbf{r} := (r_1, \cdots, r_N)^T \). Each site \( \mathbf{r} \) is also associated with \( N_{\text{orb}} \) orbital (flavors) labeled by the Greek letter \( \alpha = 1, \cdots, N_{\text{orb}} \). We define the non-interacting second-quantized Hamiltonian

\[
\hat{H} := \sum_{\mathbf{r}, \mathbf{r}'=1}^{N} \sum_{\alpha, \alpha'=1}^{N_{\text{orb}}} \hat{\psi}_{\alpha, \mathbf{r}} H_{\alpha, \mathbf{r}; \alpha', \mathbf{r}'} \hat{\psi}_{\alpha', \mathbf{r}'}^\dagger.
\]

The pair of creation (\( \hat{\psi}_{\alpha, \mathbf{r}}^\dagger \)) and annihilation operators (\( \hat{\psi}_{\alpha', \mathbf{r}'} \)) obey the fermion algebra

\[
\{ \hat{\psi}_{\alpha, \mathbf{r}}^\dagger, \hat{\psi}_{\alpha', \mathbf{r}'} \} = \delta_{\alpha, \alpha'} \delta_{\mathbf{r}, \mathbf{r}'} \text{,}
\]

\[
\{ \hat{\psi}_{\alpha, \mathbf{r}}^\dagger, \hat{\psi}_{\alpha', \mathbf{r}'}^\dagger \} = \{ \hat{\psi}_{\alpha, \mathbf{r}}, \hat{\psi}_{\alpha', \mathbf{r}'} \} = 0.
\]

Hermiticity \( \hat{H} = \hat{H}^\dagger \) is imposed by demanding that the single-particle matrix elements obey

\[
H_{\alpha, \mathbf{r}; \alpha', \mathbf{r}'} = H_{\mathbf{r}; \alpha, \mathbf{r}', \alpha'}^*.
\]

Locality, in the orbital-lattice basis, is imposed by demanding that

\[
\lim_{|\mathbf{r} - \mathbf{r}'| \to \infty} \| H_{\alpha, \mathbf{r}; \alpha', \mathbf{r}'} \| \leq \lim_{|\mathbf{r} - \mathbf{r}'| \to \infty} c \times e^{-|\mathbf{r} - \mathbf{r}'|/\ell}
\]

for some positive constant \( c \) and for some characteristic length scale \( \ell \) independent of the lattice sites \( \mathbf{r}, \mathbf{r}' = 1, \cdots, N \) and of the orbital indices \( \alpha, \alpha' = 1, \cdots, N_{\text{orb}} \). If we collect the orbital (\( \alpha \)) and lattice (\( \mathbf{r} \)) indices into a single collective index \( I \equiv (\alpha, \mathbf{r}) \), we may introduce the short-hand notation

\[
\hat{H} \equiv \sum_{I, I' \in \Omega} \hat{\psi}_{I}^\dagger H_{II'} \hat{\psi}_{I'} \equiv \hat{\psi}^\dagger \mathcal{H} \hat{\psi},
\]

where \( \mathcal{H} \) is a Hermitian \( N_{\text{tot}} \times N_{\text{tot}} \) matrix with \( N_{\text{tot}} = N_{\text{orb}} \times N \) and \( \Omega \) is the set

\[
\Omega := \{1, \cdots, N_{\text{orb}}\} \times \Lambda
\]

obtained by taking the Cartesian product of the set of orbitals with the set of lattice points.

The Hermitian matrix \( \mathcal{H} \) has \( N_{\text{tot}} \) pairs of eigenvalues and eigenvectors \((\varepsilon_I, u_I)\) that are defined by demanding
that
\[ H \psi_I = \varepsilon_I \psi_I, \quad \psi_I^\dagger \psi_{I'} = \delta_{I,I'}, \] (6.3a)
for \( I, I' = 1, \ldots, N_{\text{tot}} \). With the help of the unitary matrix
\[ U = (\nu_1, \ldots, \nu_{N_{\text{tot}}}), \] (6.3b)
we may represent the single-particle Hamiltonian \( H \) as the diagonal matrix
\[ U^\dagger H U = \text{diag} (\varepsilon_1, \ldots, \varepsilon_{N_{\text{tot}}}) \] (6.3c)
The canonical transformation
\[ \hat{\psi}_I = \sum_{J=1}^{N_{\text{tot}}} U_{IJ} \hat{\chi}_J, \] (6.3d)
gives the representation
\[ \hat{H} = \sum_{I=1}^{N_{\text{tot}}} \hat{\chi}_I^\dagger \varepsilon_I \hat{\chi}_I. \] (6.3e)
The ground state of \( N_f \) fermions is then the Fermi sea
\[ |\Psi_{\text{FS}}\rangle := \prod_{I=1}^{N_f} \hat{\chi}_I^\dagger |0\rangle, \quad \hat{\chi}_I |0\rangle = 0, \] (6.4a)
whereby we have assumed that
\[ I < I' \implies \varepsilon_I \leq \varepsilon_{I'}. \] (6.4b)

**Entanglement spectrum of the equal-time one-point correlation matrix**

We seek to partition the Fock space \( \mathcal{F} \), on which the non-interacting Hamiltonian \( \hat{H} \) defined by Eq. (6.3) acts, into two Fock subspace, which we denote by \( \mathcal{F}_A \) and \( \mathcal{F}_B \), according to the tensorial decomposition
\[ \mathcal{F} = \mathcal{F}_A \otimes \mathcal{F}_B. \] (6.5)

Two ingredients are necessary to define the subspaces \( \mathcal{F}_A \) and \( \mathcal{F}_B \). We need a state from \( \mathcal{F} \) that is a single Slater determinant. It is for this quality that we choose the ground state (6.4). We need a basis, that we choose to be the orbital-lattice basis defined by the representation (6.3).
Following Ref. [173], we start from the equal-time one-point correlation function (matrix)

\[ C_{IJ} := \left\langle \Psi_{FS} \left| \hat{\psi}_I \hat{\psi}_J \right| \Psi_{FS} \right\rangle, \quad I, J = 1, \ldots, N_{\text{tot}}. \]  

(6.6)

Insertion of Eqs. (6.4) and (6.3d) delivers

\[ C_{IJ} = N_f \sum_{I' = 1}^{N_f} U_{II'} U_{JI'} \equiv N_f \sum_{I' = 1}^{N_f} \langle \upsilon_{I'} | I \rangle \langle J | \upsilon_{I'} \rangle, \]

(6.7)

where \( I, J = 1, \ldots, N_{\text{tot}} \). We define the \( N_{\text{tot}} \times N_{\text{tot}} \) correlation matrix \( C \) by its matrix elements (6.7). One then verifies that

\[ C^\dagger = C, \quad C^2 = C, \]

(6.8)

i.e., the correlation matrix \( C \) is a Hermitian projector. The last equality of Eq. (6.7) introduces the bra and ket notation of Dirac for the single-particle eigenstates of \( \mathcal{H} \) defined by Eq. (6.3) to emphasize that this projector is nothing but the sum over all the single-particle eigenstates of \( \mathcal{H} \) that are occupied in the ground state. Thus, all \( N_{\text{tot}} \) eigenvalues of the correlation matrix \( C \) are either the numbers 0 or 1. When it is convenient to shift the eigenvalues of the correlation matrix from the numbers 0 or 1 to the numbers \( \pm 1 \), this is achieved through the linear transformation

\[ Q_{IJ} := I - 2C_{IJ}, \quad I, J = 1, \ldots, N_{\text{tot}}. \]

(6.9)

The occupied single-particle eigenstates of \( \mathcal{H} \) in the ground state of \( \hat{H} \) are all eigenstates of \( Q \) with eigenvalue \(-1\).

The unoccupied single-particle eigenstates of \( \mathcal{H} \) in the ground state of \( \hat{H} \) are all eigenstates of \( Q \) with eigenvalue \(+1\).

In other words, \( Q \) is the difference between the projector onto the unoccupied single-particle eigenstates of \( \mathcal{H} \) in the ground state of \( \hat{H} \) and the projector onto the occupied single-particle eigenstates of \( \mathcal{H} \) in the ground state of \( \hat{H} \). As such \( Q \) possesses all the symmetries of \( \mathcal{H} \) and all the spectral symmetries of \( \mathcal{H} \).

We denote the \( N_{\text{tot}} \)-dimensional single-particle Hilbert space on which the correlation function \( C \) acts by \( \mathcal{H} \). The labels \( A \) and \( B \) for the partition are introduced through the direct sum decomposition

\[ \mathcal{H} = \mathcal{H}_A \oplus \mathcal{H}_B, \]

(6.10a)

whereby \( A \) and \( B \) are two non-intersecting subsets of the set \( \Omega \) defined by Eq. (6.2f) such that

\[ \Omega = A \cup B, \quad A \cap B = \emptyset, \]

(6.10b)
and
\[ \mathcal{C} = \begin{pmatrix} C_A & C_{AB} \\ C_{AB}^\dagger & C_B \end{pmatrix}, \quad Q = \begin{pmatrix} I - 2C_A & -2C_{AB} \\ -2C_{AB}^\dagger & I - 2C_B \end{pmatrix}. \] (6.10c)

By construction, the \( N_A \times N_A \) block \( C_A \) and the \( N_B \times N_B \) block \( C_B \) are Hermitian matrices. These blocks inherit the property that their eigenvalues are real numbers bounded between the numbers 0 and 1 from \( C \) being a Hermitian projector. We call the set
\[ \sigma(C_A) := \{ \zeta_\iota \mid \exists v_\iota \in \mathbb{C}^{N_A}, \ C_A v_\iota = \zeta_\iota v_\iota, \ i = 1, \cdots, N_A \} \] (6.11a)
of single-particle eigenvalues of the block \( C_A \) the entanglement spectrum of the correlation matrix \( C \). Any eigenvalue from \( \sigma(C_A) \) obeys
\[ 0 \leq \zeta_\iota \leq 1, \quad \iota = 1, \cdots, N_A. \] (6.11b)
The single-particle eigenvalues of the \( N_A \times N_A \) Hermitian matrix \( C_A \) can be shifted from their support in the interval \([0, 1]\) to the interval \([-1, +1]\) through the linear transformation
\[ Q_A := I - 2C_A. \] (6.12)

We refer to the set \( \sigma(Q_A) \) of single-particle eigenvalues of the \( N_A \times N_A \) Hermitian matrix \( Q_A \) as the entanglement spectrum of the correlation matrix \( Q \), which we shall abbreviate as the entanglement spectrum.

It is shown in Ref. [173] that there exists a \( N_A \times N_A \) block Hermitian matrix (entanglement Hamiltonian) \( H^E \equiv (H^E_{K,L})_{K,L \in A} \) with the positive definite operator
\[ \hat{\rho}_A := \frac{e^{-\sum_{K',L' \in A} \hat{\psi}_{K'}^\dagger H^E_{K,L'} \hat{\psi}_{L}'}}{\text{tr}_A \ e^{-\sum_{K',L' \in A} \hat{\psi}_{K'}^\dagger H^E_{K,L'} \hat{\psi}_{L}'}} \] (6.13a)
whose domain of definition defines the Fock space \( \mathfrak{F}_A \) such that the block \( C_A \) from the correlation matrix (6.10c) is
\[ C_A = \left( \text{tr}_A \hat{\rho}_A \hat{\psi}_K^\dagger \hat{\psi}_L \right)_{K,L \in A}. \] (6.13b)
The positive definite matrix \( \hat{\rho}_A \) is the reduced density matrix acting on the Fock space \( \mathfrak{F}_A \) obtained by tracing the degrees of freedom from the Fock space \( \mathfrak{F}_B \) in the density matrix
\[ \hat{\rho}_{FS} := |\Psi_{FS}\rangle \langle \Psi_{FS}| \] (6.13c)
whose domain of definition is the Fock space \( \mathcal{F} \).

It is also shown in Ref. [173] that the single-particle spectrum \( \sigma(C_A) \) of the \( N_A \times N_A \) Hermitian matrix \( C_A \) is related to the single-particle spectrum \( \sigma(H) \) of the \( N_A \times N_A \) Hermitian matrix \( H^E \) by

\[
\zeta_i = \frac{1}{e^{\varpi_i} + 1}, \quad i = 1, \ldots, N_A.
\] (6.14)

Equation (6.14) states that the dependence of the eigenvalue \( \zeta_i \) of \( C_A \) on the eigenvalue \( \varpi_i \) of \( H \) is the same as that of the Fermi-Dirac function on the single-particle energy \( \varpi_i \) when the inverse temperature is unity and the chemical potential is vanishing in units for which the Boltzmann constant is unity. Equation (6.14) is a one-to-one mapping between \( \sigma(C_A) \) and \( \sigma(H) \).

Equation (6.14) allows to express the entanglement entropy

\[
S_{ee}^A := -\text{tr}_A \left( \hat{\rho}_A \ln \hat{\rho}_A \right)
\] (6.15)

of the reduced density matrix \( \hat{\rho}_A \) in terms of \( \sigma(C_A) \) through

\[
S_{ee}^A = -\sum_{i=1}^{N_A} \left[ \zeta_i \ln \zeta_i + (1 - \zeta_i) \ln(1 - \zeta_i) \right].
\] (6.16)

Zero modes of \( C_A \) are eigenstates of \( C_A \) with vanishing eigenvalues. The vector space spanned by the zero modes of \( C_A \) is denoted by \( \text{ker}(C_A) \) in linear algebra. We conclude that the zero modes of \( C_A \) do not contribute to the entanglement entropy.

**Equal-time one-point correlation matrix and SUSY QM**

It was observed in Refs. [157] and [158] that the \( 2 \times 2 \) block structure (6.10c) on the Hermitian correlation matrix \( C \) defined by its matrix elements (6.6) is compatible with the condition (6.8) that the correlation matrix is a projector if and only if the four conditions

\[
C_A^2 - C_A = -C_{AB} C_A^\dagger, \quad C_B^2 - C_B = -C_{AB}^\dagger C_{AB},
\] (6.17a)

\[
Q_A C_{AB} = -C_{AB} Q_B, \quad C_{AB}^\dagger Q_A = -Q_B C_{AB}^\dagger,
\] (6.17b)

\[
C_{AB}^\dagger Q_B = -Q_B^\dagger C_{AB}, \quad C_{AB} Q_A = -C_{AB}^\dagger Q_B,
\] (6.17c)

53
hold. Here, the $N_A \times N_A$ matrix $Q_A$ was defined in Eq. (6.12) and we have introduced the $N_B \times N_B$ matrix $Q_B := \mathbb{I} - 2 C_B$.

The family of $2N_{\text{susy}} + 1$ operators

\[
\left( \hat{Q}_1^\dagger, \hat{Q}_1, \ldots, \hat{Q}_{N_{\text{susy}}}^\dagger, \hat{Q}_{N_{\text{susy}}}, \hat{H} \right)
\] (6.18a)

acting on a common Hilbert space realizes the graded Lie algebra of supersymmetric quantum mechanics (SUSY QM) if and only if

\[
\left[ \hat{Q}_i^\dagger, \hat{H} \right] = \left[ \hat{Q}_i, \hat{H} \right] = 0,
\] (6.18b)

\[
\left\{ \hat{Q}_i, \hat{Q}_j^\dagger \right\} = \delta_{i,j} \hat{H},
\] (6.18c)

holds for $i,j = 1, \ldots, N_{\text{susy}}$. SUSY QM is realized when $\hat{H}$, which is Hermitian by construction because of Eq. (6.18c), can be identified with a Hamiltonian. Conversely, a Hamiltonian in quantum mechanics is supersymmetric if there exists a factorization of the form (6.18). It is then convention to call the operators $\hat{Q}_i^\dagger$ and $\hat{Q}_i$ with $i = 1, \ldots, N_{\text{susy}}$ supercharges owing to Eq. (6.18b). We are going to show that the algebra (6.17) is an example of SUSY QM with $N_{\text{susy}} = 1$ in disguise.

To this end, we define the $N_A \times N_A, N_B \times N_B, N_A \times N_B$, and $N_B \times N_A$ block matrices

\[
S_A := \mathbb{I} - Q_A^2, \quad S_B := \mathbb{I} - Q_B^2,
\] (6.19a)

\[
M^+ \equiv M^\dagger := 2 C_{AB}, \quad M^- \equiv M := 2 C_{AB}^\dagger,
\] (6.19b)

respectively. By construction, the spectrum of the Hermitian $N_A \times N_A$ matrix $S_A$ and that of the Hermitian $N_B \times N_B$ matrix $S_B$ belong to the interval $[0, 1]$. One verifies with the help of Eq. (6.17) that

\[
M^+ S_B - S_A M^+ = 0, \quad M^- S_A - S_B M^- = 0,
\] (6.20a)

\[
M^+ M^- = S_A, \quad M^- M^+ = S_B.
\] (6.20b)

We cannot close the graded Lie algebra (6.18) with the four block matrices (6.19). However, we still have the possibility to define the triplet of $N_{\text{tot}} \times N_{\text{tot}}$ matrices

\[
S_{\text{susy}} = \begin{pmatrix} S_A & 0 \\ 0 & S_B \end{pmatrix}, \quad Q_{\text{susy}} := \begin{pmatrix} 0 & 0 \\ M & 0 \end{pmatrix},
\] (6.21)
and $Q^\dagger$. One verifies that they satisfy the graded Lie algebra
\[ [Q_{\text{susy}}, S_{\text{susy}}] = [Q^\dagger_{\text{susy}}, S_{\text{susy}}] = 0, \tag{6.22a} \]
\[ \{Q_{\text{susy}}, Q_{\text{susy}}^\dagger\} = \{Q^\dagger_{\text{susy}}, Q_{\text{susy}}^\dagger\} = 0, \tag{6.22b} \]
\[ \{Q_{\text{susy}}, Q_{\text{susy}}^\dagger\} = S_{\text{susy}}, \tag{6.22c} \]
i.e., the pair of supercharge matrices $Q^\dagger_{\text{susy}}$ and $Q_{\text{susy}}$ and the Hamiltonian matrix $S_{\text{susy}}$ realize SUSY QM with $N_{\text{tot}} = 1$.

The grading labeled by $A$ and $B$ in the definition of the matrices in Eq. (6.22) originates from the decomposition of the single particle Hilbert space $\mathcal{H}$ into the direct sum (6.10a). The matrix $S_{\text{susy}}$ is block diagonal, i.e., it does not mix the subspaces $\mathcal{H}_A$ and $\mathcal{H}_B$. The pair of matrices $Q^\dagger_{\text{susy}}$ and $Q_{\text{susy}}$ are off-diagonal with respect to the labels $A$ and $B$, i.e., they mix the subspaces $\mathcal{H}_A$ and $\mathcal{H}_B$. The matrix $M^- \equiv M$ maps $\mathcal{H}_A$ into $\mathcal{H}_B$. Its adjoint $M^+ \equiv M^\dagger$ maps $\mathcal{H}_B$ into $\mathcal{H}_A$. In the context of SUSY QM, the pair $M^-$ and $M^+$ are called intertwiner.

We are now going to show that the Eqs. (6.19), (6.21), and (6.22) imply that the number of linearly independent eigenstates of $S_{\text{susy}}$ with vanishing eigenvalues, i.e., the number of linearly independent zero modes is larger or equal to
\[ |\dim \mathcal{H}_A - \dim \mathcal{H}_B| \equiv |N_A - N_B|. \tag{6.23} \]

To see this, we assume without loss of generality that $N_A > N_B$. When the dimension $N_A$ of $\mathcal{H}_A$ is larger than the dimension $N_B$ of $\mathcal{H}_B$, $M^+$ is a rectangular matrix with more rows than columns while $M^-$ is a rectangular matrix with more columns than rows. There follows two consequences. On the one hand, the condition
\[ M^- \mathcal{H}_A = 0 \tag{6.24} \]
that defines the null space of $M^-$ necessarily admits $N_A - N_B > 0$ linearly independent solutions in $\mathcal{H}_A$, for we must solve $N_B$ equations for $N_A$ unknowns. On the other hand, the condition
\[ M^+ \mathcal{H}_B = 0 \tag{6.25} \]
that defines the null space of $M^+$ is overdetermined, for we must solve $N_A$ equations for $N_B$ unknowns. The condition
\[ S_{\text{susy}} \mathcal{H} = 0 \tag{6.26} \]
that defines the null space of \( S_{\text{susy}} \) delivers at least \( N_A - N_B > 0 \) linearly independent solutions of the form

\[
v = \begin{pmatrix} v_A \\ 0 \end{pmatrix}
\]  

(6.27)

where

\[
M^- v_A = 0.
\]  

(6.28)

As observed by Witten in Ref. [174], the number of zero modes plays an important role in SUSY QM. The number of zero modes of \( S_{\text{susy}} \) is given by the Witten index

\[
\Delta_w := \left| \text{dim ker}(M^-) - \text{dim ker}(M^+) \right| \geq |N_A - N_B|.
\]  

(6.29)

The relevance of Eq. (6.29) to the entanglement spectrum of non-interacting fermions is the main result of Sec. 6.2.1.

**Chiral symmetry of the entanglement spectrum \( \sigma(Q_A) \)**

We have seen that the existence of zero modes in the spectrum \( \sigma(S_{\text{susy}}) \) of \( S_{\text{susy}} \) defined in Eq. (6.21) is guaranteed when the dimensionalities \( N_A \) and \( N_B \) of the single-particle Hilbert spaces \( \mathcal{H}_A \) and \( \mathcal{H}_B \), respectively, are unequal. We have shown that this property is a consequence of a hidden supersymmetry. When \( N_A = N_B \), we cannot rely on SUSY QM to decide if \( 0 \in \sigma(S_{\text{susy}}) \).

The non-interacting Hamiltonian \( \hat{H} \) defined by Eq. (6.2a) in the orbital-lattice basis acts on the Fock space \( \mathcal{F} \). Let \( \mathcal{O} \) denote an operation, i.e., an invertible mapping of time, of the lattice, of the orbital degrees of freedom, or of compositions thereof. We represent this operation by either a unitary or an anti-unitary transformation on the Fock space \( \mathcal{F} \). In turn, it suffices to specify how the creation and annihilation operators defined by their algebra (6.2b) transform under the operation \( \mathcal{O} \) to represent \( \mathcal{O} \) on the Fock space \( \mathcal{F} \).

For example, the transformation law

\[
\hat{\psi}_I \rightarrow \hat{O} \hat{\psi}_I \hat{O}^\dagger \equiv \sum_{I'=1}^{N_{\text{tot}}} \mathcal{O}_{I'I} \hat{\psi}_{I'}, \quad I = 1, \cdots, N_{\text{tot}},
\]  

(6.30)

where \( \mathcal{O} = (\mathcal{O}_{I'I}) \in U(N_{\text{tot}}) \) is a unitary matrix, realizes in a unitary fashion the operation \( \mathcal{O} \). The non-interacting Hamiltonian \( \hat{H} \) defined in Eq. (6.2) and the correlation matrix \( \mathcal{C} \) defined in Eq. (6.6) obey the transformation laws

\[
\hat{H} \rightarrow \hat{O} \hat{H} \hat{O}^\dagger \Rightarrow \mathcal{H}^T \rightarrow \mathcal{O} \mathcal{H}^T \mathcal{O},
\]  

(6.31)
and
\[ C \rightarrow O^\dagger CO, \]  
(6.32)
respectively.

For comparison, the operations of time reversal \((\mathcal{O}_{\text{tr}}, \hat{O}_{\text{tr}}, O_{\text{tr}})\) and charge conjugation (that exchanges particle and holes) \((\mathcal{O}_{\text{ph}}, \hat{O}_{\text{ph}}, O_{\text{ph}})\) are anti-unitary transformations for which
\[ C \rightarrow O_{\text{tr}}^\dagger CO_{\text{tr}}, \quad O_{\text{tr}} \equiv T_{\text{tr}} K, \quad T_{\text{tr}}^{-1} = T_{\text{tr}}^\dagger, \]  
(6.33)
and
\[ C \rightarrow O_{\text{ph}}^\dagger CO_{\text{ph}}, \quad O_{\text{ph}} \equiv T_{\text{ph}} K, \quad T_{\text{ph}}^{-1} = T_{\text{ph}}^\dagger, \]  
(6.34)
respectively. Here, \( K \) is the anti-linear operation of complex conjugation.

The non-interacting Hamiltonian \( \hat{H} \) has \( \mathcal{O} \) as a symmetry if and only if
\[ \hat{O} \hat{H} \hat{O}^\dagger = \hat{H} \iff \mathcal{H}^T = O^\dagger H^T O, \]  
(6.35)
Moreover, if we assume the transformation law
\[ |\Psi_{FS}\rangle \rightarrow e^{i\Theta} |\Psi_{FS}\rangle, \quad 0 \leq \Theta < 2\pi, \]  
(6.36)
for the ground state (6.4), i.e., if we assume that the ground state does not break spontaneously the symmetry (6.35), then
\[ C = O^\dagger CO \iff Q = O^\dagger Q O. \]  
(6.37a)
We want to derive what effect condition (6.37a) has on the entanglement spectrum \( \sigma(Q_A) \), i.e., when the direct sum decompositions (6.10) and
\[ O = \begin{pmatrix} O_A & O_{AB} \\ O_{BA} & O_B \end{pmatrix} \in U(N_{\text{tot}}), \]  
(6.37b)
hold for two special cases.

First, we assume that
\[ O = \begin{pmatrix} O_A & 0 \\ 0 & O_B \end{pmatrix}, \quad O_A \in U(N_A), \quad O_B \in U(N_B). \]  
(6.38a)
This situation arises when the operation \( \mathcal{O} \) is compatible with the partitioning encoded by the two subsets \( A \) and \( B \) of
\[ \Omega \text{ in the sense that} \]

\[ A = \theta A, \quad B = \theta B. \quad (6.38b) \]

If so, condition (6.37) simplifies to

\[ Q_A = O_A^\dagger Q_A O_A, \quad (6.39a) \]
\[ C_{AB} = O_A^\dagger C_{AB} O_B, \quad (6.39b) \]
\[ Q_B = O_B^\dagger Q_B O_B. \quad (6.39c) \]

Thus, the \( N_A \times N_A \) Hermitian block matrices \( C_A \) and \( Q_A = I - 2C_A \) inherit the symmetry obeyed by the \( N_{\text{tot}} \times N_{\text{tot}} \) Hermitian matrix \( \mathcal{H} \) when Eq. (6.38) holds.

Second, we assume that

\[ N_A = N_B = N_{\text{tot}}/2 \quad (6.40a) \]

and

\[ \mathcal{O} = \begin{pmatrix} 0 & O_{AB} \\ O_{BA} & 0 \end{pmatrix}, \quad O_{AB}, O_{BA} \in U(N_{\text{tot}}/2). \quad (6.40b) \]

This situation arises when the operation \( \theta \) interchange the two subsets \( A \) and \( B \) of \( \Omega \),

\[ A = \theta B, \quad B = \theta A. \quad (6.40c) \]

If so, condition (6.37) simplifies to

\[ Q_A = O_{BA}^\dagger Q_B O_{BA}, \quad (6.41a) \]
\[ C_{AB} = O_{BA}^\dagger C_{BA} O_{AB} \quad (6.41b) \]
\[ Q_B = O_{AB}^\dagger Q_A O_{AB}. \quad (6.41c) \]

We are going to combine Eq. (6.41) with Eq. (6.17). Multiplication of Eq. (6.41a) from the right by Eq. (6.41b) gives the relation

\[ Q_A C_{AB} = O_{BA}^\dagger Q_B C_{BA} O_{AB}, \quad (6.42) \]

while multiplication of Eq. (6.41b) from the right by Eq. (6.41c) gives the relation

\[ C_{AB} Q_B = O_{BA}^\dagger C_{BA} Q_A O_{AB}. \quad (6.43) \]
We may then use Eq. (6.17b) to infer that
\[ Q_A C_{AB} = - C_{AB} Q_B. \] (6.44)

A second use of Eq. (6.41c) delivers
\[ Q_A C_{AB} = - C_{AB} O^\dagger_{AB} Q_A O_{AB}. \] (6.45)

We introduce the auxiliary \((N_{\text{tot}}/2) \times (N_{\text{tot}}/2)\) matrix
\[ \Gamma_{\theta A} := C_{AB} O^\dagger_{AB}, \] (6.46a)
whose domain and co-domain are the single-particle Hilbert space \(\mathcal{H}_A\). We may then rewrite Eq. (6.45) as the vanishing anti-commutator
\[ \{Q_A, \Gamma_{\theta A}\} = 0. \] (6.46b)

The same manipulations with the substitution \(A \leftrightarrow B\) deliver
\[ \{Q_B, \Gamma_{\theta B}\} = 0, \] (6.46c)
where
\[ \Gamma_{\theta B} := C_{BA} O^\dagger_{BA}. \] (6.46d)

Equations (6.46b) and (6.46c) are the main result of Sec. 6.2.1.

An important consequence of Eq. (6.46b) is that the spectra \(\sigma(Q_A)\) and \(\sigma(Q_B)\), are endowed with a symmetry not necessarily present in the spectrum \(\sigma(\mathcal{H})\) when Eqs. (6.35), (6.37), and (6.40) hold. This spectral symmetry is reminiscent of the so-called chiral symmetry, the property that a single-particle Hamiltonian anti-commutes with a unitary operator, although, here, the operator \(\Gamma_{\theta}\) is not necessarily unitary. If we assume that \(C_{AB}\) is an invertible \((N_{\text{tot}}/2) \times (N_{\text{tot}}/2)\) matrix, to any pair \((1 - 2 \zeta \neq 0, v_i)\) that belongs to \(\sigma(Q_A)\), the image pair \((-1 + 2 \zeta \neq 0, \Gamma_{\theta} v_i)\) also belongs to \(\sigma(Q_A)\), and conversely. We shall say that the entanglement spectrum \(\sigma(Q_A)\) is chiral symmetric, when Eqs. (6.35), (6.37), (6.40) hold with \(\Gamma_{\theta}\) defined in Eq. (6.46d) invertible.

Here, we shall consider a regular \(d\)-dimensional lattice \(\Lambda\), say a Bravais lattice. We denote with \(P_\parallel \subset \mathbb{R}^d\) the plane with the coordinates
\[ \begin{pmatrix} r_\parallel \\ 0 \end{pmatrix}, \quad r_\parallel \in \mathbb{R}^n, \quad n = 1, \ldots, d - 1. \] (6.47a)
We denote with $P_\perp \subset \mathbb{R}^d$ the plane with the coordinates
\[
\begin{pmatrix}
0 \\
r_\perp
\end{pmatrix}, \quad r_\perp \in \mathbb{R}^{d-n}, \quad n = 1, \cdots, d - 1.
\]
(6.47b)

Any lattice point $r$ from $\Lambda$ can be written as
\[
r \equiv \begin{pmatrix} r_\parallel \\ r_\perp \end{pmatrix} \in \mathbb{R}^d.
\]
(6.47c)

We define the operation of reflection $R$ about the plane $P_\perp \subset \mathbb{R}^d$ by
\[
r \equiv \begin{pmatrix} r_\parallel \\ r_\perp \end{pmatrix} \rightarrow R \equiv \begin{pmatrix} -r_\parallel \\ +r_\perp \end{pmatrix},
\]
(6.48a)
\[
\hat{\psi}_{\alpha,r} \rightarrow \hat{R} \hat{\psi}_{\alpha,r} \hat{R}^\dagger \equiv \sum_{\beta=1}^{N_{\text{orb}}} R_{\alpha\beta} \hat{\psi}_{\beta,Rr},
\]
(6.48b)

for any $\alpha = 1, \cdots, N_{\text{orb}}$ and $r \in \Lambda$. We define the operation of parity (inversion) $P$ by
\[
r \rightarrow P \equiv -r,
\]
(6.49a)
\[
\hat{\psi}_{\alpha,r} \rightarrow \hat{P} \hat{\psi}_{\alpha,r} \hat{P}^\dagger \equiv \sum_{\beta=1}^{N_{\text{orb}}} P_{\alpha\beta} \hat{\psi}_{\beta,Pr},
\]
(6.49b)

for any $\alpha = 1, \cdots, N_{\text{orb}}$ and $r \in \Lambda$.

Even though we may impose on the non-interacting Hamiltonian (6.2) the conditions of translation and point-group symmetries when the lattice $\Lambda$ is regular, a partitioning (6.10) might break these symmetries, for it involves lattice degrees of freedom. We seek a partitioning that preserves translation invariance within the “plane” (6.47b) that is normal to the “plane” (6.47a). With this partition in mind, we first perform the Fourier transformations
\[
\mathcal{H}_{I,I'}(k_\perp) := \frac{1}{N_\perp} \sum_{r_\perp,r'_\perp} e^{ik_\perp \cdot (r_\perp - r'_\perp)} \mathcal{H}_{I,r_\perp,r'_\perp},
\]
(6.50a)
and
\[
\mathcal{C}_{I,I'}(k_\perp) := \frac{1}{N_\perp} \sum_{r_\perp,r'_\perp} e^{ik_\perp \cdot (r_\perp - r'_\perp)} \mathcal{C}_{I,r_\perp,r'_\perp},
\]
(6.50b)
on the single-particle Hamiltonian (6.2c) and equal-time one-point correlation matrix (6.6), respectively, where
\[ I \equiv (\alpha, r_\parallel), \quad I' \equiv (\alpha', r'_\parallel), \] (6.50c)
and \( N_\perp \) is the number of lattice sites in \( \Lambda \) holding a suitably chosen \( r_\parallel \) fixed. For some suitably chosen \( r_\perp \) held fixed, we may then define the non-intersecting partitioning of the set
\[ \Omega := \left\{ (\alpha, r_\parallel) \left| \alpha = 1, \cdots, N_{\text{orb}}, \left( \begin{array}{c} r_\parallel \\ r_\perp \end{array} \right) \in \Lambda \right. \right\} \] (6.50d)
into
\[ A = \mathcal{R} B = \mathcal{P} B \] (6.50e)
and
\[ B = \mathcal{R} A = \mathcal{P} A. \] (6.50f)
The discussion in Sec.6.2.1 is now applicable for each \( k_\perp \) separately, i.e., Eq. (6.17) becomes
\[ C_A^2(k_\perp) - C_A(k_\perp) = -C_{AB}(k_\perp) C_{AB}^\dagger(k_\perp), \] (6.51a)
\[ Q_A(k_\perp) C_{AB}(k_\perp) = -C_{AB}(k_\perp) Q_B(k_\perp), \] (6.51b)
\[ C_{AB}^\dagger(k_\perp) Q_A(k_\perp) = -Q_B(k_\perp) C_{AB}^\dagger(k_\perp), \] (6.51c)
\[ C_B^2(k_\perp) - C_B(k_\perp) = -C_{AB}^\dagger(k_\perp) C_{AB}(k_\perp). \] (6.51d)
We impose the symmetry conditions
\[ \mathcal{R}^\dagger C(k_\perp) \mathcal{R} = C(+k_\perp), \] (6.52a)
\[ \mathcal{P}^\dagger C(k_\perp) \mathcal{P} = C(-k_\perp), \] (6.52b)
where \( \mathcal{R} \) and \( \mathcal{P} \) are unitary representations of the actions of the operations of reflection \( \mathcal{R} \) and parity (inversion) \( \mathcal{P} \) on the labels (6.50c) for each \( k_\perp \) separately, respectively. We assume that \( N_A = N_B \), for which it is necessary that the dimensionality \( d \) of the lattice is even with the pair of orthogonal planes spanned by \( r_\parallel \) and \( r_\perp \) each \((d/2)\)-
We then conclude Sec. 6.2.1 with the identities

\[ \{Q_A(k_{\perp}), \Gamma_R(k_{\perp})\} = 0, \tag{6.53a} \]
\[ Q_A(k_{\perp}) \Gamma_R(k_{\perp}) + \Gamma_R(k_{\perp}) Q_A(-k_{\perp}) = 0, \tag{6.53b} \]

where \( \Gamma_R(k_{\perp}) \) and \( \Gamma_P(k_{\perp}) \) are not assumed invertible for each \( k_{\perp} \) separately.

**Equal-time one-point correlation matrix and \( \mathcal{P} \mathcal{C} \mathcal{T} \) symmetry**

Any local quantum field theory with a Hermitian Hamiltonian for which Lorentz invariance is neither explicitly nor spontaneously broken must preserve the composition (\( \mathcal{P} \mathcal{C} \mathcal{T} \)) of parity (\( \mathcal{P} \)), charge conjugation (\( \mathcal{C} \)), and time-reversal (\( \mathcal{T} \)), even though neither \( \mathcal{P} \), nor \( \mathcal{C} \), nor \( \mathcal{T} \) need to be separately conserved. \([175]\) The \( \mathcal{P} \mathcal{C} \mathcal{T} \) theorem implies the existence of antiparticles. It also implies that any composition of two out of the triplet of transformations \( \mathcal{P}, \mathcal{C}, \) and \( \mathcal{T} \) is equivalent to the third. \([176,178]\) Consequently, the \( \mathcal{P} \mathcal{C} \mathcal{T} \) theorem predicts that the \( \mathcal{T} \) symmetry is violated by the weak interactions. A direct observation for the violation of the \( \mathcal{T} \) symmetry by the weak interaction has been reported in Ref. \([179]\).\]

The \( \mathcal{P} \mathcal{C} \mathcal{T} \) theorem does not hold anymore after relaxing the condition of Lorentz invariance. The effective Hamiltonians used in condensed matter physics generically break Lorentz invariance. However, the extent to which \( \mathcal{P}, \mathcal{C}, \) and \( \mathcal{T} \) are separately conserved is not to be decided as a matter of principle but depends on the material and the relevant energy scales in condensed matter physics. For example, the effects of the earth magnetic field or those of cosmic radiation are for most practical purposes irrelevant to the properties of materials in condensed matter physics. A non-relativistic counterpart to charge conjugation symmetry holds in a mean-field treatment of superconductivity. Inversion symmetry, the non-relativistic counterpart to symmetry under parity, is common to many crystalline states of matter. The effective Hamiltonian of electrons in magnetically inert materials preserves time-reversal symmetry in the absence of an external magnetic field. Conversely, the effective Hamiltonian of electrons in the presence of magnetic impurities in metals or if the crystalline host is magnetic break explicitly time-reversal symmetry.

It has become clear in the last eight years that the notion of symmetry protected phases of matter is useful both theoretically and experimentally in condensed matter physics. It has first lead to a classification for the possible insulating phases of electrons that are adiabatically connected to Slater determinants. \([180,185]\) Some of the predicted insulating phases have then been observed in suitable materials. For each insulating phase, there exists a non-interacting many-body Hamiltonian \( \hat{H} \) that is smoothly connected to all Hamiltonians describing this insulating phase by local unitary transformations. \([154]\) This classification depends on the dimensionality of space and on the presence or absence of

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the following three discrete (i.e., involutive) symmetries. There is the symmetry of \( \hat{H} \) under time reversal \( \hat{O}_{\text{tr}} \),

\[
[\hat{H}, \hat{O}_{\text{tr}}] = 0, \quad \hat{O}_{\text{tr}}^2 = \pm 1. \tag{6.54}
\]

There is the spectral symmetry of \( \hat{H} \) under an anti-unitary transformation (particle-hole) \( \hat{O}_{\text{ph}} \),

\[
\{ \hat{H}, \hat{O}_{\text{ph}} \} = 0, \quad \hat{O}_{\text{ph}}^2 = \pm 1. \tag{6.55}
\]

There is the spectral symmetry of \( \hat{H} \) under a unitary transformation (chiral) \( \hat{O}_{\text{ch}} \),

\[
\{ \hat{H}, \hat{O}_{\text{ch}} \} = 0. \tag{6.56}
\]

There are two distinct insulating phases characterized by the presence or absence of the chiral spectral symmetry when both time reversal and particle-hole symmetry are broken. There are another eight distinct insulating phases when both time reversal and particle-hole symmetry are satisfied. For a fixed dimension of space, five of the ten insulating phases support gapless extended boundary states in geometries with open boundaries. Moreover, these three discrete symmetries can be augmented by discrete (involutive) symmetries that enforce reflection or mirror symmetries resulting in a rearrangement of which of the five insulating phases supporting gapless extended boundary states.

The single-particle matrix \( Q \) defined in Eq. (6.9) inherits from the single-particle matrix \( H \) defined by Eq. (6.3) any one of the three symmetries

\[
[Q, O_{\text{tr}}] = 0, \quad O_{\text{tr}}^2 = \pm 1, \tag{6.57a}
\]

\[
\{ Q, O_{\text{ph}} \} = 0, \quad O_{\text{ph}}^2 = \pm 1, \tag{6.57b}
\]

\[
\{ Q, O_{\text{ch}} \} = 0, \tag{6.57c}
\]

with \( O_{\text{ch}} \) implementing the chiral transformation and \( O_{\text{ch}} \) its single-particle representation, \( O_{\text{ph}} \) implementing the particle-hole transformation and \( O_{\text{ph}} \) its single-particle representation, and \( O_{\text{tr}} \) implementing reversal of time and \( O_{\text{tr}} \) its single-particle representation, respectively. Here, we are assuming that there exists a partition

\[
\Omega = A \cup B, \quad A \cap B = \emptyset, \tag{6.57d}
\]

that obeys

\[
A = \sigma \ A, \quad B = \sigma \ B, \tag{6.57e}
\]
with $\theta = \theta_{\text{tr}}, \theta_{\text{ph}}, \theta_{\text{ch}}$, when the time-reversal symmetry or the particle-hole or the chiral spectral symmetries of $Q$ are inherited from those of $H$.

Conservation of $\mathcal{PCT}$, as occurs in a relativistic local quantum-field theory, implies that the operations of parity $\mathcal{P}$, charge conjugation $\mathcal{C}$, and time-reversal $\mathcal{T}$ are not independent. The composition of any two of them is equivalent to the third one.

Even though $\mathcal{PCT}$ may not be conserved for the non-interacting Hamiltonian $H$ defined in Eq. (6.3), its correlation matrix $Q$ defined in Eq. (6.9) or its entanglement matrix $Q_A$ defined in Eq. (6.12) may obey a weaker form of a $\mathcal{PCT}$-like relation as we now illustrate by way of two examples.

Case when $\mathcal{P}$ is equivalent to $\mathcal{T}$: When the parity (inversion) transformation $\mathcal{P}$ is a symmetry of $H$, there exists a $\Gamma_{\mathcal{P}A}$ such that, by Eq. (6.46b), it anti-commutes with $Q_A$, i.e.,

$$\{Q_A, \Gamma_{\mathcal{P}A}\} = 0.$$

(6.58)

If we also assume that there exists a particle-hole transformation $O_{\text{ph}}$ (an anti-unitary transformation) that anti-commutes with with $Q_A$ (e.g., if $H$ is the Bogoliubov-de-Gennes Hamiltonian of a superconductor), i.e.,

$$\{Q_A, O_{\text{ph}}\} = 0,$$

(6.59)

it then follows that the composition

$$O_{\text{tr}} := O_{\text{ph}} \Gamma_{\mathcal{P}A}$$

(6.60)

is an anti-linear transformation that commutes with $Q_A$, i.e.,

$$[Q_A, O_{\text{tr}}] = 0.$$

(6.61)

The symmetry of $H$ under parity and the spectral symmetry of $H$ under particle-hole transformation have delivered an effective anti-linear symmetry of $Q_A$.

Case when $\mathcal{C}$ is equivalent to $\mathcal{T}$: We assume that $H$ defined in Eq. (6.3) anti-commutes with the conjugation of charge $\mathcal{C}$ represented by $O_{\text{ph}}$, while it commutes with reversal of time $\mathcal{T}$ represented by $O_{\text{tr}}$. We also assume that the partition (6.57d) obeys Eq. (6.57e) when $\theta$ is $\theta_{\text{ph}}$ or $\theta_{\text{tr}}$, i.e.,

$$O_{\text{ph}} = \left( \begin{array}{cc} O_{\text{ph}A} & 0 \\ 0 & O_{\text{ph}B} \end{array} \right), \quad O_{\text{tr}} = \left( \begin{array}{cc} O_{\text{tr}A} & 0 \\ 0 & O_{\text{tr}B} \end{array} \right).$$

(6.62)
We define
\[ \mathcal{O}_{\text{ch}} := \mathcal{O}_{\text{ph}} \mathcal{O}_{\text{tr}}, \quad \mathcal{O}_{\text{ch}} = \begin{pmatrix} \mathcal{O}_{\text{ch}A} & 0 \\ 0 & \mathcal{O}_{\text{ch}B} \end{pmatrix}. \] (6.63)

It follows that \( \mathcal{O}_{\text{ch}} \) is unitary, obeys Eq. (6.57e), and anti-commutes with \( \mathcal{H} \). Hence, we may interpret \( \mathcal{O}_{\text{ch}} \) as an effective chiral transformation. The symmetries and spectral symmetries of \( \mathcal{H} \) are passed on to \( \mathcal{Q} \) defined in Eq. (6.9).

In particular,
\[ \mathcal{O}_{\text{ch}} \mathcal{Q} = -\mathcal{Q} \mathcal{O}_{\text{ch}}. \] (6.64)

We make the additional assumption that \( h_A \) and \( h_B \) are isomorphic and that the action of \( \mathcal{O}_{\text{ch}A} \) on \( h_A \) is isomorphic to that of \( \mathcal{O}_{\text{ch}B} \) on \( h_B \). If so, we write
\[ \mathcal{O}_{\text{ch}A} \cong \mathcal{O}_{\text{ch}B} \cong \mathcal{O}_{\text{ch}}, \quad \mathcal{O}_{\text{ch}} = \begin{pmatrix} \mathcal{O}_{\text{ch}} & 0 \\ 0 & \mathcal{O}_{\text{ch}} \end{pmatrix}. \] (6.65)

Equation (6.64) then gives four conditions,
\[ \mathcal{O}_{\text{ch}} Q_A = -Q_A \mathcal{O}_{\text{ch}}, \] (6.66a)
\[ \mathcal{O}_{\text{ch}} C_{AB} = -C_{AB} \mathcal{O}_{\text{ch}}, \] (6.66b)
\[ \mathcal{O}_{\text{ch}} C_{BA} = -C_{BA} \mathcal{O}_{\text{ch}}, \] (6.66c)
\[ \mathcal{O}_{\text{ch}} Q_B = -Q_B \mathcal{O}_{\text{ch}}. \] (6.66d)

With the help of Eq. (6.17), one verifies that
\[ (\mathcal{O}_{\text{ch}} C_{BA}) Q_A = -\mathcal{O}_{\text{ch}} Q_B C_{BA} = Q_B (\mathcal{O}_{\text{ch}} C_{BA}), \] (6.67a)
\[ (\mathcal{O}_{\text{ch}} C_{BA}) C_{AB} = C_{BA} (\mathcal{O}_{\text{ch}} C_{BA}), \] (6.67b)
\[ (C_{AB} \mathcal{O}_{\text{ch}}) C_{BA} = C_{AB} (\mathcal{O}_{\text{ch}} C_{BA}), \] (6.67c)
\[ (C_{AB} \mathcal{O}_{\text{ch}}) Q_B = -C_{AB} Q_B \mathcal{O}_{\text{ch}} = Q_A (C_{AB} \mathcal{O}_{\text{ch}}). \] (6.67d)

This should be compared with Eq. (6.41). We conclude with the observation that there exists the transformation
\[ \mathcal{O}_{\text{eff}} := \begin{pmatrix} 0 & C_{AB} \mathcal{O}_{\text{ch}} \\ \mathcal{O}_{\text{ch}} C_{BA} & 0 \end{pmatrix}. \] (6.68)
that commutes with $Q$.

$$[Q, O_{\text{eff}}] = 0. \tag{6.69}$$

The spectral symmetry of $H$ under a particle-hole transformation and the symmetry of $H$ under time reversal have conspired to provide $Q$ with a symmetry under the transformation $O_{\text{eff}}$.

### 6.2.2 Interacting fermions

We consider a many-body Hamiltonian acting on the Fock space $\mathcal{F}$ introduced in Eq. (6.3) that describes $N_f$ interacting fermions. Its normalized ground state is

$$|\Psi\rangle := \sum_{n=1}^{2^{N_{\text{tot}}}} \sum_{n_1^{(n)}=0,1} \cdots \sum_{n_{N_{\text{tot}}}^{(n)}=0,1} \delta_{n_1^{(n)} + \cdots + n_{N_{\text{tot}}}^{(n)} N_f} \times c^{(\Psi)}_{n_1^{(n)} \cdots n_{N_{\text{tot}}}^{(n)}} |n_1^{(n)} \cdots n_{N_{\text{tot}}}^{(n)}\rangle. \tag{6.70a}$$

The Slater determinant

$$\langle n_1^{(n)}, \cdots, n_{N_{\text{tot}}}^{(n)} | := \prod_{I=1}^{N_{\text{tot}}} \langle 0 | \left(\hat{\chi}_I\right)^{n_I^{(n)}}, \tag{6.70b}$$

has $c^{(\Psi)}_{n_1^{(n)} \cdots n_{N_{\text{tot}}}^{(n)}}$ as its overlap with the ground state $|\Psi\rangle$.

In the presence of interactions, the equal-time one-point correlation function (matrix)

$$C_{IJ} := \langle \Psi | \hat{\psi}_I^\dagger \hat{\psi}_J | \Psi \rangle, \quad I, J = 1, \cdots, N_{\text{tot}}, \tag{6.71}$$

does not convey anymore the same information as the density matrix

$$\hat{\rho}_\Psi := |\Psi\rangle \langle \Psi|, \quad \langle \Psi| \Psi \rangle = 1. \tag{6.72a}$$

In particular, Eq. (6.71) does not encode the full information contained in the reduced density matrices

$$\hat{\rho}_\Psi^{(A)} := \text{tr}_{\mathcal{F}_B} \hat{\rho}_\Psi \tag{6.72b}$$

and

$$\hat{\rho}_\Psi^{(B)} := \text{tr}_{\mathcal{F}_A} \hat{\rho}_\Psi, \tag{6.72c}$$

where we have defined the partition in Eqs. (6.5) and (6.10).

We seek a useful representation of the reduced density matrices (6.72b) and (6.72c) and how they might be related.
by symmetries of the interacting Hamiltonian. To this end, we assign the labels $\mu_A = 1, \cdots, \dim \mathcal{F}_A$ and $\mu_B = 1, \cdots, \dim \mathcal{F}_B$ to any orthonormal basis $\{ |\Psi^{(A)}_{\mu_A}\rangle \}$ and $\{ |\Psi^{(B)}_{\mu_B}\rangle \}$ that span the Fock spaces $\mathcal{F}_A$ and $\mathcal{F}_B$, respectively. Without loss of generality, we assume $\dim \mathcal{F}_A \geq \dim \mathcal{F}_B$. We may write the expansion

$$|\Psi\rangle = \sum_{\mu_A=1}^{\dim \mathcal{F}_A} \sum_{\mu_B=1}^{\dim \mathcal{F}_B} D_{\mu_A \mu_B} |\Psi^{(A)}_{\mu_A}\rangle \otimes |\Psi^{(B)}_{\mu_B}\rangle$$  

(6.73)

with the overlaps $D_{\mu_A \mu_B} \in \mathbb{C}$ defining the matrix elements of the $\dim \mathcal{F}_A \times \dim \mathcal{F}_B$ matrix $D$.

At this stage, we make use of the singular value decomposition

$$D = U \Sigma V^\dagger$$  

(6.74a)

with

$$U = (U_{\mu_A \mu_A'})$$  

(6.74b)

a $\dim \mathcal{F}_A \times \dim \mathcal{F}_A$ unitary matrix,

$$\Sigma = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \ddots & \cdots & \vdots \\ \vdots & \ddots & \ddots & \sigma_R \\ 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \quad 0 < \sigma_1 \leq \cdots \leq \sigma_R,$$

(6.74c)

a $\dim \mathcal{F}_A \times \dim \mathcal{F}_B$ rectangular diagonal matrix of rank $R \leq \dim \mathcal{F}_B$, and

$$V = \left(V_{\mu_B \mu_B'}\right)$$  

(6.74d)

a $\dim \mathcal{F}_B \times \dim \mathcal{F}_B$ unitary matrix.

With the help of Eq. (6.74), we have the Schmidt decomposition:

$$|\Psi\rangle = \sum_{\nu=1}^{R} \sigma_\nu |\tilde{\Psi}^{(A)}_{\nu}\rangle \otimes |\tilde{\Psi}^{(B)}_{\nu}\rangle$$  

(6.75a)
where
\[ |\tilde{\Psi}_\nu^{(A)} \rangle := \sum_{\mu_A=1}^{\dim F_A} U_{\mu_A \nu} |\Psi^{(A)}_{\mu_A} \rangle \]  
(6.75b)
and
\[ |\tilde{\Psi}_\nu^{(B)} \rangle := \sum_{\mu_B=1}^{\dim F_B} V^*_{\mu_B \nu} |\Psi^{(B)}_{\mu_B} \rangle. \]  
(6.75c)

The singular values \( \{ \sigma_\nu \} \equiv \sigma(\Sigma) \) of the rectangular matrix \( \Sigma \) are non-negative and obey the normalization condition
\[ \sum_{\nu=1}^{\mathcal{R}} \sigma^2_\nu = 1 \]  
(6.75d)
owing to the facts that the ground state (6.70) is normalized to one and that the basis of \( \tilde{\mathcal{F}}_A \) and \( \tilde{\mathcal{F}}_B \) are chosen orthonormal.

In the basis (6.75),
\[ \hat{\rho}_\Psi := \sum_{\nu=1}^{\mathcal{R}} \sum_{\nu'=1}^{\mathcal{R}} \sigma_\nu \sigma_{\nu'} |\tilde{\Psi}_\nu^{(A)} \rangle \langle \tilde{\Psi}_\nu^{(A)} | \otimes |\tilde{\Psi}_\nu^{(B)} \rangle \langle \tilde{\Psi}_\nu^{(B)} | \]  
(6.76a)
and the reduced density matrices (6.72b) and (6.72c) become the spectral decompositions
\[ \hat{\rho}^{(A)}_\Psi := \sum_{\nu=1}^{\mathcal{R}} \sigma^2_\nu |\tilde{\Psi}_\nu^{(A)} \rangle \langle \tilde{\Psi}_\nu^{(A)} | \]  
(6.76b)
and
\[ \hat{\rho}^{(B)}_\Psi := \sum_{\nu=1}^{\mathcal{R}} \sigma^2_\nu |\tilde{\Psi}_\nu^{(B)} \rangle \langle \tilde{\Psi}_\nu^{(B)} |, \]  
(6.76c)
respectively. The reduced density matrices \( \hat{\rho}^{(A)}_\Psi \) and \( \hat{\rho}^{(B)}_\Psi \) are explicitly positive semi-definite. They share the same non-vanishing eigenvalues
\[ 0 < \sigma^2_\nu \equiv e^{-\omega_\nu}, \quad 0 \leq \omega_\nu < \infty, \quad \nu = 1, \cdots, \mathcal{R}, \]  
(6.76d)
each of which can be interpreted as the probability for the ground state (6.70) to be in the orthonormal basis state \( |\tilde{\Psi}_\nu^{(A)} \rangle \otimes |\tilde{\Psi}_\nu^{(B)} \rangle \).

As we did with Eq. (6.40a), we assume that
\[ \dim \tilde{\mathcal{F}}_A = \dim \tilde{\mathcal{F}}_B = \mathcal{D}. \]  
(6.77a)
Hence, \( \dim \mathcal{F}_A \) and \( \dim \mathcal{F}_B \) are isomorphic. This means that \( \hat{\Gamma}_{AB} : \mathcal{F}_B \rightarrow \mathcal{F}_A \) defined by

\[
\hat{\Gamma}_{AB} := \sum_{\nu=1}^{\mathcal{D}} |\tilde{\Psi}_\nu^{(B)}\rangle \langle \tilde{\Psi}_\nu^{(A)}|
\]  

(6.77b)

and \( \hat{\Gamma}_{BA} : \mathcal{F}_A \rightarrow \mathcal{F}_B \) defined by

\[
\hat{\Gamma}_{BA} := \sum_{\nu=1}^{\mathcal{D}} |\tilde{\Psi}_\nu^{(A)}\rangle \langle \tilde{\Psi}_\nu^{(B)}|
\]  

(6.77c)

are linear one-to-one maps. One verifies that

\[
\hat{\Gamma}_{AB}^{-1} = \hat{\Gamma}_{BA} = \hat{\Gamma}_{AB}^\dagger,
\]

(6.78a)

\[
\hat{\rho}_\psi^{(A)} = \hat{\Gamma}_{AB} \hat{\rho}_\psi \hat{\Gamma}_{AB}^\dagger, \quad \hat{\rho}_\psi^{(B)} = \hat{\Gamma}_{BA} \hat{\rho}_\psi \hat{\Gamma}_{BA}^\dagger.
\]

(6.78b)

We conclude Sec. 6.2.2 with a counterpart for interacting fermions of the spectral symmetry (6.46). We assume that the operation \( \mathcal{O} \) under which the partition is interchanged,

\[
A = \mathcal{O} B, \quad B = \mathcal{O} A,
\]

(6.79)

is represented by the unitary map \( \mathcal{O} : \mathcal{F}_A \rightarrow \mathcal{F}_B \) defined either by

\[
|\tilde{\Psi}_\nu^{(B)}\rangle_{\mathcal{O}} := \sum_{\nu'=1}^{\mathcal{R}} \mathcal{O}_{\nu\nu'} |\tilde{\Psi}_\nu^{(A)}\rangle,
\]

(6.80a)

or by its inverse \( \mathcal{O}^\dagger : \mathcal{F}_B \rightarrow \mathcal{F}_A \) defined by

\[
|\tilde{\Psi}_\nu^{(A)}\rangle =: \sum_{\nu'=1}^{\mathcal{R}} \mathcal{O}_{\nu'\nu}^* |\tilde{\Psi}_\nu^{(B)}\rangle_{\mathcal{O}},
\]

(6.80b)

whereby

\[
\sum_{\nu'=1}^{\mathcal{R}} \mathcal{O}_{\nu\nu''}^* \mathcal{O}_{\nu'\nu''} = \delta_{\nu,\nu''}
\]

(6.80c)

with \( \nu, \nu', \nu'' = 1, \cdots, \mathcal{R} \).

By Eq. (6.76b),

\[
\left( \hat{\rho}_\psi^{(A)} \right)_{\mathcal{O}} := \sum_{\nu, \nu', \nu''=1}^{\mathcal{R}} \sigma_{\nu}^z \mathcal{O}_{\nu\nu'}^* \mathcal{O}_{\nu'\nu''} |\tilde{\Psi}_\nu^{(B)}\rangle \langle \tilde{\Psi}_\nu^{(B)}|_{\mathcal{O}}
\]

(6.81)
If we impose the symmetry constraint
\[
\sum_{\nu=1}^{\mathcal{R}} \sigma_\nu^2 O_{\nu',\nu} O_{\nu'',\nu} = \begin{cases} 
\sigma_\nu^2 \delta_{\nu',\nu''}, & \text{if } \nu' = 1, \ldots, \mathcal{R}, \\
0, & \text{otherwise},
\end{cases}
\]
(6.82a)

(i.e., \(O^\dagger \Sigma O = \Sigma\)), we conclude that
\[
\left(\hat{\rho}_\Psi^{(A)}\right)_\Theta = \sum_{\nu=1}^{\mathcal{R}} \sigma_\nu^2 |\tilde{\Psi}_\nu^{(B)}\rangle_\Theta \langle \tilde{\Psi}_\nu^{(B)}| \equiv \hat{\rho}_\Psi^{(B)}
\]
(6.82b)

We can combine Eqs. (6.78) and (6.82) as follows. Given are the interacting Hamiltonian \(\hat{H}\) acting on the Fock space \(\mathcal{F}\) defined in the orbital-lattice basis, the density matrix \(\hat{\rho}_\Psi\) for the ground state \(|\Psi\rangle\) of \(\hat{H}\), the partition \(\mathcal{F} = \mathcal{F}_A \otimes \mathcal{F}_B\), and the reduced density matrix \(\hat{\rho}_\Psi^{(A)}\) and \(\hat{\rho}_\Psi^{(B)}\) acting on the Fock spaces \(\mathcal{F}_A\) and \(\mathcal{F}_B\) with \(\dim \mathcal{F}_A = \dim \mathcal{F}_B\), respectively. Let \(\hat{\Sigma}\) represent the action by conjugation on the space of operators of the matrix (6.74c). Let \(\hat{\mathcal{O}}\) represent the action by conjugation on the space of operators of the matrix \(\mathcal{O}\) with the matrix elements (6.80). Let

\[
\hat{\Xi} := \Gamma_{BA} \hat{\mathcal{O}}
\]
(6.83)

and assume the symmetry
\[
\hat{\mathcal{O}}^\dagger \hat{\Sigma} \hat{\mathcal{O}} = \hat{\Sigma}.
\]
(6.84)

The symmetry
\[
\hat{\rho}_\Psi^{(A)} = \hat{\Xi}^\dagger \hat{\rho}_\Psi^{(A)} \hat{\Xi}
\]
(6.85)

obeyed by the reduced density matrix then follows.

### 6.3 Physical versus entangling boundaries, spectral gap, and locality

Topological band insulators are insulators with two equivalent properties in the thermodynamic limit. If the discrete symmetry of time reversal, or the spectral symmetries of charge conjugation or chirality are imposed together with periodic boundary conditions, the bundle of Bloch states making up a ground state defines a quantized index, i.e., a number that does not change if the bundle of Bloch states is changed smoothly without violating the discrete symmetries or closing the band gap. The quantization of this index is a topological attribute of the occupied bands that is protected by certain discrete symmetries. If open boundary conditions are imposed instead of periodic ones, mid-gap single-particle states that are exponentially localized on the boundaries descend from the continuum of occupied
and unoccupied Bloch states. These boundary states are protected, i.e., robust to perturbations that are compliant with the discrete symmetries, change smoothly Bloch states, and do not close the band gap. This equivalence between a topological index when periodic boundary conditions are imposed and protected boundary states when open boundary conditions are imposed is an example of a bulk-edge correspondence.

We shall call the boundaries in position space (i.e., in the orbital basis) that are selected by imposing open boundary conditions on the single-particle Hamiltonian \( \mathcal{H} \) defined in Eq. (6.2) the physical boundaries. It is possible to define another class of boundaries in position space (i.e., in the orbital basis) by performing the partitioning (6.10). We call the boundaries that separate the lattice labels of the orbital basis in set \( A \) from those in set \( B \) the entangling boundaries. The number of entangling boundaries depends on whether periodic, open, or mixed boundary conditions are imposed. For a one-dimensional lattice such as the one shown in Fig. 6.2(a), choosing periodic boundary conditions selects no physical boundaries as is shown in the left panel of Fig. 6.2(b), while it selects two identical entangling boundaries as is shown in the left panel of Fig. 6.2(c). On the other hand, choosing open boundary conditions selects two identical physical boundaries as is shown in the right panel of Fig. 6.2(b), while it selects one physical boundary and one entangling boundary as is shown in the right panel of Fig. 6.2(c).

It has been proposed that the existence of protected single-particle states that are localized at the entangling boundaries, i.e., protected entangling boundary states, is a more refined signature for topological band insulators than the existence of protected physical boundary states. Indeed, it is argued that the existence of protected physical boundary states implies the existence of protected entangling boundary states for a suitable partition. [148, 153, 157, 158] However, the converse is known not to hold. For example, three-dimensional inversion symmetric topological insulators have been constructed such that the physical boundary states can be gapped out by inversion-symmetric perturbations, while the entangling boundary states remain gapless. [157, 158]

### 6.3.1 Spectral gap and locality of the equal-time one-point correlation matrix

In this context, the following observations are crucial. On the one hand, none of the results of Sec. 6.2 are sensitive to the presence or absence of a spectral gap \( \Delta \) separating the Slater determinant entering the definition (6.6) of the equal-time one-point correlation matrix \( C \) from all excited states when periodic boundary conditions are imposed. On the other hand, the stability analysis from Secs. 6.4–6.7 only makes sense if \( \Delta > 0 \), since the exponential decay of the boundary states away from the boundaries is controlled by the characteristic length \( \xi \propto 1/\Delta \). Consequently, the overlap of two boundary states localized on disconnected boundaries a distance \( N \) apart vanishes exponentially fast as the thermodynamic limit \( N \to \infty \) is taken, i.e., the matrix elements \( C_{IJ} \) in Eq. (6.6) also decay exponentially fast if the pair of repeat unit cells in the collective labels \( I \) and \( J \) are a distance larger than \( \xi \) apart. In particular, the matrix elements entering the upper-right block \( C_{AB} \) in Eq. (6.10) and those entering the transformation (6.46d) are
Figure 6.1: (a) The real line \( \{ x \in \mathbb{R} \} \) is partitioned into two open sets, the negative axis \( A \) and the positive axis \( B \). The boundary between \( A \) and \( B \) is the origin at \( x = 0 \), a compact set. This boundary is the entangling boundary of the real line, a connected set. The real line has two disconnected physical boundaries at \( x = -\infty \) and \( x = +\infty \). The inversion about the origin \( x \mapsto -x \) is smooth, exchanges \( A \) and \( B \), and has the entangling boundary as its unique fixed point. The map \( x \mapsto -1/x \) is not smooth at the origin, exchanges \( A \) and \( B \), and has no fixed point. The real line is the limit \( r \to 0 \) of a cylinder with the radius \( r \) embedded in three-dimensional Cartesian space. (b) The circle \( \{ \theta \in [0, 2\pi] \} \) can be interpreted as the compactification of the real line if the physical boundaries at \( x = -\infty \) and \( x = +\infty \) are identified with the angle \( \theta = \pi \) and the origin of the real line is identified as the angle \( \theta = 0 \), respectively. These are two disconnected compact sets. The inversion about \( \theta = 0 \) defined by \( \theta \mapsto -\theta \) is smooth, exchanges \( A \) and \( B \), and has the two distinct fixed points \( \theta = 0 \) and \( \theta = \pi \). The inversion about \( \theta = \pi \) defined by \( \theta \mapsto \pi - \theta \) is smooth, leaves \( A \) (\( B \)) invariant as a set, and exchanges \( \theta = 0 \) and \( \theta = \pi \). The translation defined by \( \theta \mapsto \pi + \theta \), the composition of the two previous inversions, is smooth, exchanges \( A \) and \( B \), and has no fixed points. A circle of radius \( R \) is the limit \( r \to 0 \) of a ring torus obtained by revolving a circle of radius \( r \) in three-dimensional Cartesian space about an axis coplanar with the circle a distance \( R > r \) apart from the center of mass of the revolving circle.

... suppressed exponentially in magnitude if they correspond to two repeat unit cells a distance larger than \( \xi \) apart. It is only because of the presence of a spectral gap above the ground state of the Hamiltonian \( \mathcal{H} \) defined in Eq. (6.2) that \( C \) defined in Eq. (6.10) inherits from \( \mathcal{H} \) its locality in the orbital basis.

### 6.3.2 Spectral gap and locality of the spectral symmetry (6.46d)

In the remaining of this chapter, we shall be concerned with exploring the effects of the spectral symmetry (6.46d) on the entanglement spectra when a single-particle bulk spectral gap \( \Delta \) guarantees that the equal-time one-point correlation matrices (6.6) and (6.9) are local for bulk-like separations, i.e., their matrix elements in the position basis can be bounded from above by the exponential factor \( a \exp(-b|r|\Delta) \) where \( a \) and \( b \) are some numerical factor of order unity and \( |r| \geq 1/\Delta \) (in units with the Planck constant set to \( \hbar = 1 \) and the speed of light set to \( c = 1 \)) is the bulk-like distance in space of the lattice degrees of freedom entering the bra and ket. In other words, we seek to understand how the spectral properties of the block \( Q_A \) of the equal-time one-point correlation matrix defined in Eq. (6.9) are affected by the assumption that a symmetry operation \( \Theta \) conspires with the partition of the degrees of freedom of the single-particle Hilbert space so as to obey Eq. (6.40), i.e., the map

\[
\Gamma_{\Theta_A} : \mathcal{F}_A \mapsto \mathcal{F}_A
\]

defined by the matrix multiplication \( \Gamma_{\Theta_A} := C_{AB} \Theta_{AB}^\dagger \) anti-commutes with \( Q_A \).
Typically, the symmetry operation $O$ is a point-group symmetry, say an inversion or reflection symmetry. Hence, we shall assume that the symmetry operation $O$ is not local. The spectral symmetry of $Q_A$ generated by $\Gamma_{O,A}$ allows to draw definitive conclusions on the existence of protected zero modes in the entanglement spectrum $\sigma(Q_A)$ only if $\Gamma_{O,A}$ is a local operation for bulk-like separations. For this reason, we devote section 6.3.2 to studying the conditions under which $\Gamma_{O,A}$ is local for bulk-like separations.

We shall consider two geometries for simplicity. Either we impose on $d$-dimensional space the geometry of a cylinder by imposing periodic boundary conditions in all $(d-1)$ directions in space while imposing open boundary conditions for the last direction. Or we impose on $d$-dimensional space the geometry of a torus by imposing periodic boundary conditions to all $d$ directions in space. When space is one dimensional, the cases of cylindrical and torus geometry are illustrated in Fig. 6.1(a) and 6.1(b), respectively.

For a cylindrical geometry, as illustrated in Fig. 6.1(a), there are two disconnected compact physical boundaries at $x = \pm \infty$ and one compact entangling boundary at $x = 0$, where $x$ is the non-compact coordinate along the cylinder axis. We choose the symmetry operation $O$ to be the mirror operation $x \mapsto -x$ that leaves the compact entangling boundary at $x = 0$ point-wise invariant, while it exchanges the two disconnected compact physical boundaries at $x = \pm \infty$. The matrix elements of $\Gamma_{O,A}$ involving bra and kets with lattice degrees of freedom a distance $|r| \gg 1/\Delta$ away from the entangling boundary at $x = 0$ are exponentially suppressed by the factor $\exp(-b|r|\Delta)$ originating from $C_{AB}^\dagger$. Hence, $\Gamma_{O,A}$ is a local operator for bulk-like separations that generates a spectral symmetry on $Q_A$ without mixing boundary states localized on disconnected boundaries (whether physical or entangling).

For a torus geometry, as illustrated in Fig. 6.1(a), there are two disconnected compact entangling boundaries at $\theta = 0$ and $\theta = \pi$. On the one hand, we may choose the symmetry operation $O$ to be the mirror operation $\theta \mapsto -\theta$ that leaves the compact entangling boundary at $\theta = 0$ and $\theta = \pi$ point-wise invariant. The matrix elements of $\Gamma_{O,A}$ involving bra and kets with lattice degrees of freedom a distance $|r| \gg 1/\Delta$ away from the entangling boundaries at $\theta = 0$ and $\theta = \pi$ are exponentially suppressed by the factor $\exp(-b|r|\Delta)$ originating from $C_{AB}^\dagger$. Hence, $\Gamma_{O,A}$ is again a local operator for bulk-like separations that generates a spectral symmetry on $Q_A$ without mixing boundary states localized on disconnected entangling boundaries. On the other hand, we may choose the symmetry operation $O$ to be the mirror operation $\theta \mapsto \pi + \theta$ that exchanges the compact entangling boundary at $\theta = 0$ and $\theta = \pi$. Hence, $\Gamma_{O,A}$ is not a local operator for it mixes with an amplitude of order unity boundary states localized on disconnected entangling boundaries separated by an arbitrary distance. Hence, even though $\Gamma_{O,A}$ generates a spectral symmetry of the entanglement spectrum of $Q_A$, it cannot be used to deduce any stability properties of the zero modes localized on the boundaries.

Sections 6.4-6.7 are devoted to the stability analysis of entangling boundary states by way of examples in one and two dimensions. This stability analysis requires distinguishing the nature of the boundaries in the partition (6.10), for
Figure 6.2: (a) Hoppings of fermions between three consecutive sites $r-1$, $r$, and $r+1$ along a one-dimensional ring with four orbitals per site. A repeat unit cell is labeled by the integer $r = 1, \ldots, N$ and is pictured by a rounded rectangular frame. A unit cell contains four orbitals that are pictured by black or white discs or squares, respectively. The hopping amplitude $t + \delta t \in \mathbb{R}$ is pictured by a full connecting line. The hopping amplitude $t - \delta t \in \mathbb{R}$ is pictured by a dashed connecting line. Hopping is only possible between orbitals of the same shape but distinct colors belonging to nearest-neighbor repeat unit cell. The figure is invariant under (i) the composition of the interchange of the full and dashed lines with the interchange of the black and white filling colors with a reflection about the horizontal dash-one-dot (red) line $RH$ and (ii) the composition of the interchange of the circular and square shapes with a reflection about the vertical dash-two-dots (blue) line $RVO$ if $N$ is odd or the vertical dash-three-dots (green) line $RVE$ if $N$ is even.

(b) Periodic boundary conditions are imposed (ring geometry) on the repeat unit cells represented by filled circles in the left panel, whereas open boundary conditions are imposed (open line geometry) on the repeat unit cells in the right panel. There are two physical boundaries on either sides of the cut represented by the dashed line a distance $N$ apart. (c) Periodic boundary conditions are imposed (ring geometry) on the repeat unit cells represented by filled circles in the left panel, whereas open boundary conditions are imposed (open line geometry) on the repeat unit cells in the right panel. The partitions $A$ and $B$ are made of the unit cells above and below the dashed line, respectively. There are two identical entangling boundaries an integer distance $N/2$ apart in the left panel. There are two identical physical boundaries a distance $N$ apart in the right panel, each of which is an integer distance $N/2$ apart from a single entangling boundary.

whether these boundaries are physical or entangling depends on the choice of the boundary conditions imposed along the $d$ dimensions of space, as we have illustrated for the case of $d = 1$ in Fig. 6.2. This stability analysis also requires determining if the spectral symmetry $\Gamma_{\sigma, A}$ is local or not, as we have illustrated for the case of $d = 1$ in Fig. 6.1.

6.4 Topological insulator protected by reflection (inversion) symmetry in one dimension

6.4.1 Hamiltonian

Our first example is defined by choosing $d = 1$ and $N_{\text{orb}} = 4$ in Eq. 6.2. The lattice $\Lambda$ is one-dimensional with the lattice spacing $2a$. It is labeled by the integers $r = 1, \ldots, N$. To represent the single-particle Hamiltonian with the matrix elements (6.2d), we introduce two sets of Pauli matrices. We associate to the unit $2 \times 2$ matrix $\sigma_0$ and the
three Pauli matrices $\sigma_1$, $\sigma_2$, and $\sigma_3$ two geometrical shapes, a square or a circle, corresponding to the eigenvalues of $\sigma_3$. We associate to the unit $2 \times 2$ matrix $\tau_0$ and the three Pauli matrices $\tau_1$, $\tau_2$, and $\tau_3$ two colors, black or white, corresponding to the eigenvalues of $\tau_3$. We choose the representation

$$\hat{\psi}^\dagger_r \equiv \left( \hat{\psi}^\dagger_{\Box, r}, \hat{\psi}^\dagger_{\square, r}, \hat{\psi}^\dagger_{\bullet, r}, \hat{\psi}^\dagger_{\circ, r} \right)$$

(6.87a)

and impose periodic boundary conditions

$$\hat{\psi}^\dagger_{r+N} = \hat{\psi}^\dagger_r, \quad r = 1, \ldots, N.$$  

(6.87b)

The non-interacting Hamiltonian is then defined by

$$\hat{H} := (t + \delta t) \sum_{r=1}^N \left( \hat{\psi}^\dagger_{\Box, r+1} \hat{\psi}_{\Box, r} + \hat{\psi}^\dagger_{\square, r+1} \hat{\psi}_{\square, r} + \hat{\psi}^\dagger_{\bullet, r} \hat{\psi}_{\bullet, r} + \hat{\psi}^\dagger_{\circ, r} \hat{\psi}_{\circ, r+1} \right) + (t - \delta t) \sum_{r=1}^N \left( \hat{\psi}^\dagger_{\square, r+1} \hat{\psi}_{\Box, r} + \hat{\psi}^\dagger_{\bullet, r+1} \hat{\psi}_{\bullet, r} + \hat{\psi}^\dagger_{\circ, r} \hat{\psi}_{\circ, r+1} + \hat{\psi}^\dagger_{\circ, r} \hat{\psi}_{\circ, r+1} \right)$$

(6.87c)

in second quantization. It describes the nearest-neighbor hops of fermions with hopping amplitudes $t \pm \delta t \in \mathbb{R}$ as is illustrated in Fig. 6.2. The corresponding single-particle Hamiltonian can be written $[\tau_{\pm} := (\tau_1 \pm i\tau_2)/2]$

$$\mathcal{H}_{r, r'}(t, \delta t) := \delta_{r', r-1} \left\{ (t + \delta t) \left[ \frac{\sigma_0 + \sigma_3}{2} \otimes \tau_+ + \frac{\sigma_0 - \sigma_3}{2} \otimes \tau_- \right] 
+ (t - \delta t) \left[ \frac{\sigma_0 + \sigma_3}{2} \otimes \tau_- + \frac{\sigma_0 - \sigma_3}{2} \otimes \tau_+ \right] \right\} 
+ \delta_{r', r+1} \left\{ (t + \delta t) \left[ \frac{\sigma_0 + \sigma_3}{2} \otimes \tau_- + \frac{\sigma_0 - \sigma_3}{2} \otimes \tau_+ \right] 
+ (t - \delta t) \left[ \frac{\sigma_0 + \sigma_3}{2} \otimes \tau_+ + \frac{\sigma_0 - \sigma_3}{2} \otimes \tau_- \right] \right\}. \quad (6.87d)$$

In the Bloch basis, the single-particle Hamiltonian (6.87c) becomes

$$\mathcal{H}_{k, k'} = \mathcal{H}_k \delta_{k, k'}, \quad \mathcal{H}_k = 2t \cos k \sigma_0 \otimes \tau_1 - 2\delta t \sin k \sigma_3 \otimes \tau_2, \quad k, k' = -\pi + \frac{2\pi}{N}, \ldots, \pi, \quad (6.88a)$$

with the single-particle spectrum consisting of the two-fold degenerate pair of bands

$$\varepsilon_{\pm, k} = \pm 2|t| \sqrt{\cos^2 k + (\delta t/t)^2 \sin^2 k}. \quad (6.88b)$$
Table 6.1: The spectrum $\sigma(\tilde{H}_{\mu\nu})$ of the single-particle Hamiltonian $\tilde{H}_{\mu\nu}$, defined by Eq. (6.109) with open boundary conditions. Hamiltonian $\tilde{H}_{\mu\nu}$ is nothing but Hamiltonian $\tilde{H}$ [defined in Eq. (6.87)] perturbed additively by the term $\delta_{r,r'}\left(t/10\right)\tilde{X}_{\mu\nu}$ with $\tilde{X}_{\mu\nu} \equiv \sigma_{\mu} \otimes \tau_{\nu}$. The choices for $\tilde{X}_{\mu\nu}$ made in the first eight rows enumerate all perturbations $\mathcal{V}_{\mu\nu}$ defined by Eq. (6.109b) that enter Eq. (6.108), i.e., that preserve the symmetry under the parity of $\tilde{H}$ generated by $\mathcal{P}_{10}$. The last two rows are two examples of a perturbation $\mathcal{V}_{\mu\nu}$ that breaks parity. The entanglement spectrum $\sigma(\tilde{Q}_{\mu\nu|A})$ defined by Eq. (6.12) for the single-particle Hamiltonian $\tilde{H}_{\mu\nu}$ obeying periodic boundary conditions. The entry $\circ$ or $\times$ denotes the presence or the absence of the symmetries under parity $\mathcal{P}$, charge conjugation $\mathcal{C}$, and time reversal $\mathcal{P}$ of the perturbation $\delta_{r,r'}\left(t/10\right)\tilde{X}_{\mu\nu}$ for the first sixteen columns. In the last two columns, the entry $\circ$ or $\times$ denotes the presence or the absence, respectively, of zero modes (mid-gap) states in the spectra $\sigma(\tilde{H}_{\mu\nu})$ and $\sigma(\tilde{Q}_{\mu\nu|A})$ as determined by extrapolation to the thermodynamic limit of exact diagonalization with $N = 12$.

Consequently, the band gap

$$\Delta = 4 |\delta t|$$

(6.88c)

opens at the boundary of the first Brillouin zone for any non-vanishing $\delta t$.

### 6.4.2 Symmetries

The symmetries of the single-particle Hamiltonian defined by Eq. (6.87) are the following, for any pair of sites $r, r' = 1, \cdots, N$.

[1] Translation symmetry holds,

$$\mathcal{H}_{r, r'}(t, \delta t) = \mathcal{H}_{r+n, r'+n}(t, \delta t), \quad \forall n \in \mathbb{Z}.$$  

(6.89)

[2] When the dimerization vanishes

$$\mathcal{H}_{r, r'}(t, \delta t = 0) = t \left( \delta_{r', r-1} + \delta_{r', r+1} \right) \sigma_0 \otimes \tau_1,$$

(6.90)
the discrete symmetries

\[ 0 = \{ \mathcal{H}_{r,r'}(t, \delta t = 0), \sigma_\mu \otimes \tau_\nu \} \] (6.91a)

hold for \( \mu = 0, 1, 2, 3 \) and \( \nu = 0, 1 \), whereas the discrete spectral symmetries

\[ 0 = \{ \mathcal{H}_{r,r'}(t, \delta t = 0), \sigma_\mu \otimes \tau_\mu \} \] (6.91b)

hold for \( \mu = 0, 1, 2, 3 \) and \( \nu = 2, 3 \).

[3] For any dimerization, the transformation laws

\[ \mathcal{H}_{r,r'}(t, +\delta t) = \sigma_\mu \otimes \tau_1 \mathcal{H}_{r,r'}(t, -\delta t) \sigma_\mu \otimes \tau_1 \] (6.92a)

with \( \mu = 0, 3 \) implement the symmetry of Fig. 6.2 under the composition of the interchange of the full and dashed lines with the interchange of the black and white filling colors with a reflection about the horizontal dash-one-dot (red) line \( \mathcal{R}H \), whereas the transformation laws

\[ \mathcal{H}_{r,r'}(t, +\delta t) = \sigma_\mu \otimes \tau_1 \mathcal{H}_{r,r'}(t, +\delta t) \sigma_\mu \otimes \tau_1 \] (6.92b)

hold for \( \mu = 1, 2 \) otherwise.

[4] Let \( \mathcal{E}_R \) be the operation that interchanges site \( r_1 \) with site \( r_{N} \), site \( r_2 \) with site \( r_{N-1} \), and so on, i.e., a reflection about the vertical dash-two-dots (blue) line \( \mathcal{R}VO \) if \( N \) is odd or the vertical dash-three-dots (green) line \( \mathcal{R}VE \) if \( N \) is even. For any dimerization, the transformation laws

\[ \mathcal{H}_{r,r'}(t, \delta t) = \sigma_\mu \otimes \mathcal{E}_R \mathcal{E}_{r,r'}(t, \delta t) \sigma_\mu \otimes \tau_0 \] (6.93)

with \( \mu = 1, 2 \) are unitary symmetries, whereas the transformation laws

\[ \mathcal{H}_{r,r'}(t, \delta t) = \sigma_\mu \otimes \mathcal{E}_R \mathcal{E}_{r,r'}(t, \delta t) \sigma_\mu \otimes \tau_3 \] (6.94)

with \( \mu = 1, 2 \) are unitary spectral symmetries.

It is also instructive to derive the symmetries and spectral symmetries of the single-particle Hamiltonian 6.88 for any \( k = \pi/N, \cdots, \pi \) from the first Brillouin zone.
To this end, it is convenient to introduce the more compact notation

\[ X_{\mu\nu} := \sigma_{\mu} \otimes \tau_{\nu}, \quad \mu, \nu = 0, 1, 2, 3, \quad (6.95a) \]

for the sixteen linearly independent $4 \times 4$ Hermitian matrices that generate the unitary group $U(4)$. In the Bloch basis (6.88a),

\[ H_{k,k'} = \mathcal{H}_{k} \delta_{k,k'}, \quad \mathcal{H}_{k} = 2t \cos k X_{01} - 2 \delta t \sin k X_{32}, \quad (6.95b) \]

for $k, k' = \pi/N, \cdots, \pi$. We have taken advantage of the fact that $X_{01}$ and $X_{32}$ anti-commute to derive the band dispersions (6.88b).

There are eight matrices $X_{\mu\nu}$ with $\mu = 0, 1, 2, 3$ and $\nu = 0, 1$ that commute with $X_{01}$, there are eight matrices $X_{\mu\nu}$ with $\mu = 1, 2$ and $\nu = 1, 3$ or $\mu = 0, 3$ and $\nu = 0, 2$ that commute with $X_{32}$. This leaves the four matrices $X_{00}, X_{30}, X_{11}$, and $X_{21}$ that commute with $\mathcal{H}_{k}$ for all $k$ in the Brillouin zone.

There are eight matrices $X_{\mu\nu}$ with $\mu = 0, 1, 2, 3$ and $\nu = 2, 3$ that anti-commute with $X_{01}$, there are eight matrices $X_{\mu\nu}$ with $\mu = 1, 2$ and $\nu = 0, 2$ or $\mu = 0, 3$ and $\nu = 1, 3$ that anti-commute with $X_{32}$. This leaves the four matrices $X_{12}, X_{22}, X_{03}$, and $X_{33}$ that anti-commute with $\mathcal{H}_{k}$ for all $k$ in the Brillouin zone.

The symmetries

\[ O^{\dagger}_\mathcal{O} \mathcal{H}_{-k} O_\mathcal{O} = \mathcal{H}_{+k}, \quad (6.96a) \]
\[ O^{\dagger}_\mathcal{T} \mathcal{H}^{*}_{-k} O_\mathcal{T} = \mathcal{H}_{+k}, \quad (6.96b) \]

with

\[ O_\mathcal{O} \in \{X_{01}, X_{10}, X_{20}, X_{31}\}, \quad (6.96c) \]
\[ O_\mathcal{T} \in \{X_{00}, X_{11}, X_{21}, X_{30}\}, \quad (6.96d) \]

whereas the spectral symmetries

\[ O^{\dagger}_\mathcal{O} \mathcal{H}^{T}_{-k} O_\mathcal{O} = -\mathcal{H}_{k}, \quad (6.97a) \]
\[ O^{\dagger}_\mathcal{T} \mathcal{H}_{k} O_\mathcal{T} = -\mathcal{H}_{k}, \quad (6.97b) \]
follow. As anticipated, the set of chiral-like spectral symmetries is identical the set of particle-hole-like spectral symmetries in view of the presence of four time-reversal-like symmetries. We shall use the notation $K$ for the anti-linear operation of complex conjugation. We shall also introduce the notation

Parity: \[ P_{10} := \sigma_1 \otimes \tau_0 = +P_{10}^T, \] (6.98a)

Charge Conjugation: \[ C_{03} := \sigma_0 \otimes \tau_3 K = +C_{03}^T, \] (6.98b)

Time Reversal: \[ T_{21} := \sigma_2 \otimes \tau_1 K = -T_{21}^T, \] (6.98c)

Chirality: \[ S_{22} := \sigma_2 \otimes \tau_2 = +S_{22}^T, \] (6.98d)

say, to distinguish the operations of parity (reflection or inversion), charge conjugation (particle hole interchange), time reversal, and chirality, respectively. The symmetry under parity of $\mathcal{H}$ can be realized in four inequivalent ways. Correspondingly, we define the $4 \times 4$ matrices

Parity $\mathcal{P}$: \[ \mathcal{P}_{01}, \mathcal{P}_{10}, \mathcal{P}_{20}, \mathcal{P}_{31}, \] (6.99a)

that realize the algebra of the unit $2 \times 2$ matrix $\rho_0$ and of the three Pauli matrices $\rho_1, \rho_2, \rho_3$. The symmetry under time reversal of $\mathcal{H}$ can be realized in four inequivalent ways. Correspondingly, we define the $4 \times 4$ matrices

Time Reversal $\mathcal{T}$: \[ \mathcal{T}_{00}, \mathcal{T}_{11}, \mathcal{T}_{21}, \mathcal{T}_{30}, \] (6.99b)

that realize the algebra of $\rho_0 K, \rho_1 K, \rho_2 K$, and $\rho_3 K$. The symmetry under charge conjugation of $\mathcal{H}$ can be realized in four inequivalent ways. Correspondingly, we define the $4 \times 4$ matrices

Charge Conjugation $\mathcal{C}$: \[ \mathcal{C}_{03}, \mathcal{C}_{12}, \mathcal{C}_{22}, \mathcal{C}_{33}, \] (6.99c)

that realize the algebra of $\rho_0 K, \rho_1 K, \rho_2 K$, and $\rho_3 K$. All the possible compositions of the operations for charge conjugation and time reversal give four realizations for the chiral symmetry of $\mathcal{H}$. Correspondingly, we define the
that realize the algebra of $\rho_0$, $\rho_1$, $\rho_2$, and $\rho_3$. There are sixteen columns in Table 6.1, each of which correspond to one of these matrix operations. We shall then select 12 triplets $(P_{\mu\nu}, T_{\mu\nu}, C_{\mu\nu})$ from Eqs. (6.99) to build the rows of Table 6.2.

The single-particle Hamiltonian $\mathcal{H}$ is extremely sparse. This is reflected by it obeying the symmetries $(P_{\mu}, T_{\mu}, C_{\mu})$ with the pair $\mu$ and $\nu$ fixed by the columns from Table 6.1. In particular, $\mathcal{H}$ cannot be assigned in a unique way the symmetry under time-reversal and the spectral symmetry under charge conjugation without additional informations of microscopic origin. Identifying the symmetric space generated by $\mathcal{H}$ is thus ambiguous. Example 1, $\mathcal{H}$ can be thought of as representative of the Cartan symmetry class CI if the choice $T_{\mu\nu}$ obeying $T_{\mu\nu}^2 = +\mathbb{I}$ and $C_{\mu\nu}$ obeying $C_{\mu\nu}^2 = -\mathbb{I}$ for the symmetry under time-reversal and the spectral symmetry under charge-conjugation is dictated by a microscopic derivation of $\mathcal{H}$. Example 2, $\mathcal{H}$ can be thought of as representative of the symmetry class DIII if the choice $T_{\mu\nu}$ obeying $T_{\mu\nu}^2 = -\mathbb{I}$ and $C_{\mu\nu}$ obeying $C_{\mu\nu}^2 = +\mathbb{I}$ for the symmetry under time-reversal and the spectral symmetry under charge-conjugation is dictated by a microscopic derivation of $\mathcal{H}$. Example 3, $\mathcal{H}$ can be thought of as representative of the Cartan symmetry class BDI if the choice $T_{\mu\nu}$ obeying $T_{\mu\nu}^2 = +\mathbb{I}$ and $C_{\mu\nu}$ obeying $C_{\mu\nu}^2 = +\mathbb{I}$ for the symmetry under time-reversal and the spectral symmetry under charge-conjugation is dictated by a microscopic derivation of $\mathcal{H}$. In fact, all complex Cartan symmetry classes AI, BDI, D, DIII, AII, CII, C, and CI are obtained from perturbing $\mathcal{H}$ under the condition that either a symmetry under time reversal or a spectral symmetry under charge conjugation is imposed by a microscopic derivation of $\mathcal{H}$. Finally, if a microscopic derivation of $\mathcal{H}$ does not prevent perturbations that break all the symmetries under time reversal and all the spectral symmetries under charge conjugations from Table 6.1 then the remaining two real Cartan symmetry classes A and AIII are realized.

### 6.4.3 Partition, topological numbers, and zero modes

It is time to turn our attention to the topological properties of the single-particle Hamiltonian $\mathcal{H}$ defined by its matrix elements (6.87) or (6.88) in the orbital basis or in the Bloch basis, respectively.

The representation (6.88) demonstrates that the single-particle Hamiltonian $\mathcal{H}$ is reducible for all $k$ in the Brillouin zone,

$$
\mathcal{H} = \bigoplus_{n=1}^{N} \mathcal{H}_{\pi n/N},
$$

$$
\mathcal{H}_k = \mathcal{H}_k^{(+)} \oplus \mathcal{H}_k^{(-)},
$$

80
Table 6.2: The first column gives all possible combinations for the triplet of symmetries \( P_{\mu\nu}, T_{\mu\nu}, \) and \( C_{\mu\nu} \), from Table 6.1 that are compatible with the Cartan symmetry class CI defined by the conditions \( T_{\mu\nu}^2 = +1 \) and \( C_{\mu\nu}^2 = -1 \). The second column gives for each row the most general perturbation \( V_{\mathcal{P},\mathcal{T},\mathcal{C}} \) that obeys the triplet of symmetries \( \{\mathcal{P}, \mathcal{T}, \mathcal{C}\} \) on any given row. The third column gives the doublet \( (\eta, \eta_{\mathcal{P}}) \in \{-, +\} \times \{-, +\} \) where the sign \( \eta \) is defined by \( \mathcal{P} \mathcal{T} \mathcal{P} = \eta \mathcal{T} \mathcal{P} \) and similarly for \( \eta_{\mathcal{P}} \). The fourth column is an application of the classification for the symmetry-protected topological band insulators in one-dimensional space derived in Refs. [160] and [161] (Table VI from Ref. [161] was particularly useful). The topological index \( \mathbb{Z} \) and \( 0 \) correspond to topologically nontrivial and trivial bulk phases, respectively. The entry \( \circ \) or \( \times \) in the last column denotes the presence or absence of zero modes in the spectrum \( \sigma(Q_{\mu\nu, \mathcal{A}}) \) as is explained in Sec. 6.4.4 and verified by numerics.

where the \( 4 \times 4 \) Hermitian matrices \( H_k^{(+)} \) and \( H_k^{(-)} \) are isomorphic to the \( 2 \times 2 \) Hermitian matrices

\[
H_k^{(+)} := 2t \cos k \tau_1 - 2\delta t \sin k \tau_2 \tag{6.100c}
\]

and

\[
H_k^{(-)} := 2t \cos k \tau_1 + 2\delta t \sin k \tau_2, \tag{6.100d}
\]

respectively.

The reducibility (6.100) defines the partition (6.10) for the one-dimensional example (6.88). For simplicity, we take the thermodynamic limit \( N \to \infty \) with \( N = 2M \) so that we may define

\[
\mathcal{D}_A := \bigoplus_{n=1}^{M} \bigoplus_{\mu, \nu = \pm} |\chi^{(\mu)}_{\mu; \nu; \pi n/2M} \rangle \langle \chi^{(\mu)}_{\nu; \mu; \pi n/2M} |	ag{6.101a}
\]

and

\[
\mathcal{D}_B := \bigoplus_{n=M+1}^{2M} \bigoplus_{\mu, \nu = \pm} |\chi^{(\mu)}_{\mu; \nu; \pi n/2M} \rangle \langle \chi^{(\mu)}_{\nu; \mu; \pi n/2M} |. \tag{6.101b}
\]

Here, \( \chi^{(+)}_{\pm k} \) and \( \chi^{(+)}_{+ k} \) are the pair of eigenstates with eigenvalues \( \varepsilon^{(+)}_{-k} \leq \varepsilon^{(+)}_{+k} \) of \( H_k^{(+)} \). Similarly, \( \chi^{(-)}_{-k}, \chi^{(-)}_{+k} \), and \( \varepsilon^{(-)}_{-k} \leq \varepsilon^{(-)}_{+k} \) denote the eigenstates and their eigenenergies from the lower and upper bands of \( H_k^{(-)} \). This partition
satisfies [recall Eq. (6.98)]

\[ \mathcal{P} A = B, \quad \mathcal{P} B = A, \quad (6.102a) \]
\[ \mathcal{C} A = A, \quad \mathcal{C} B = B, \quad (6.102b) \]
\[ \mathcal{T} A = A, \quad \mathcal{T} B = B, \quad (6.102c) \]
\[ \mathcal{S} A = A, \quad \mathcal{S} B = B. \quad (6.102d) \]

Hamiltonian (6.100c) describes a single-particle that hops between sites labeled by ■ and □ in Fig. 6.2 with the uniform hopping amplitude \( t \) and the staggered hopping amplitude \( \delta t \). Hamiltonian (6.100d) describes a single-particle that hops between sites labeled by • and ◦ in Fig. 6.2 with the uniform hopping amplitude \( t \) and the staggered hopping amplitude \( \delta t \).

If we take the thermodynamic limit

\[ N, N_f \to \infty \quad (6.103a) \]

holding the fermion density

\[ N_f/N = 1 \quad (6.103b) \]

fixed, we find the non-vanishing winding numbers

\[ W_{FS}^{(+)} = -W_{FS}^{(-)} := \frac{i}{2\pi} \oint d k \chi^{(+)}\uparrow(k) \left( \frac{\partial \chi^{(+)\downarrow}}{\partial k} \right)(k) \quad (6.104) \]

for any non-vanishing dimerization \( \delta t \). Owing to the reducibility of \( \mathcal{H}_k \), the winding number \( W_{FS} \) for the single-particle eigenstates making up the Fermi sea of \( \mathcal{H}_k \) is

\[ W_{FS} = W_{FS}^{(+)} + W_{FS}^{(-)} = 0 \quad (6.105) \]

for any non-vanishing dimerization \( \delta t \). The non-vanishing values of the winding numbers endow each of the single-particle Hamiltonians \( H^{(+)} \) and \( H^{(-)} \) with a topological attribute. The single-particle Hamiltonian \( \mathcal{H} \) is topologically trivial as its winding number vanishes.

The very definition of the winding numbers (6.104) and (6.105) requires twisted boundary conditions and a spectral gap between the Fermi sea and all many-body excitations.

With open boundary conditions, two zero-dimensional boundaries at \( r - 1 \) and \( r \) follow from setting all hopping amplitudes between site \( r - 1 \) and \( r \) in Fig. 6.2 to zero, i.e., erasing the connecting full and dashed lines from Fig. 6.2 that intersect the vertical line \( RVE \). In such an open geometry, the winding numbers (6.104) and (6.105)
are ill defined. However, the bulk-edge correspondence implies the existence of mid-gap states (zero modes) that are localized at the boundaries (if the thermodynamic limit is taken with open boundary conditions), whenever the winding numbers \(6.104\) are non-vanishing (if the thermodynamic limit is taken with twisted boundary conditions). There are four such zero modes, a pair of zero modes for each boundary. On any given boundary, one of the zero modes localized on this boundary originates from \(H^{(+)}_{r,r'}\), while the other originates from \(H^{(-)}_{r,r'}\). These four zero modes are eigenstates of either \(X_{03} + X_{33}\) or \(X_{03} - X_{33}\). As a set, they are protected against any perturbation that anti-commutes with \(X_{03}\) and \(X_{33}\), i.e., they are protected against any linear combination of \(X_{01}, X_{02}, X_{31},\) and \(X_{32}\). [We have verified by exact diagonalization that the zero modes in \(\sigma(H)\) are indeed robust to the perturbations \(X_{01}, X_{02}, X_{31},\) or \(X_{32}\).]

It is believed that the existence of protected gapless boundary states, when taking the thermodynamic limit with open boundary conditions for a topological band insulator with Hamiltonian \(H\), implies the existence of protected gapless boundary states in the entanglement spectrum of \(Q_A\) for a suitable partition of the form \(6.10\), when taking the thermodynamic limit with closed boundary conditions for the equal-time one-point correlation matrix \(Q\). \[148, 153, 157, 158\]

We have verified by exact diagonalization that this is also the case when we take the thermodynamic limit \(6.103\) of \(H\) defined by Eq. \(6.100\) with an even number of sites \(N = 2M\) and with the partition defined by Eq. \(6.101\). The spectra for \(H\) and \(Q_A\) are shown in Fig.\[6.3\](a) for \(\delta t = t\) and \(N = 12\). In both spectra, there are four zero modes within an exponential accuracy resulting from finite-size corrections. In the case of \(H\), a pair of zero modes is exponentially localized at one physical boundary a distance \(2M\) apart from the second pair of zero modes localized on the opposite boundary. In the case of \(Q_A\), a pair of zero modes is exponentially localized at the boundary with \(B\) to the left of \(A\) a distance \(M\) apart from the second pair of zero modes exponentially localized at the boundary with \(A\) to the left of \(B\). The exponential decay of the zero modes away from their boundary is inversely proportional to the band gap of \(H\) when periodic boundary conditions are imposed.

We observe that the existence of zero modes in the spectrum of \(Q_A\) does not imply the existence of zero modes in the spectrum of \(H\). For example, if we shift the spectrum of \(H\) defined in Eq. \(6.100\) in a uniform way by adding a chemical potential smaller than the band gap, we immediately lose the zero modes. However, all single-particle eigenstates are unperturbed by the chemical potential, for it enters as a perturbation that commutes with \(H\). Consequently, neither \(Q\), nor \(Q_A\), nor their spectra depend on the chemical potential. In particular, the spectrum of \(Q_A\) with a non-vanishing chemical potential contains the very same four zero modes that are present when the chemical potential vanishes.

The question we are after is the following. Are the four zero modes of \(H_{r,r'}(t,\delta t)\), that are localized at both ends of an open chain, stable against perturbations that (i) commute with a reflection from Table \[6.1\] and (ii) have a characteristic energy that is small relative to the unperturbed band gap? Similarly, how stable are the four zero modes
Figure 6.3: Energy spectra $\sigma(\tilde{H}_{\mu\nu})$ in units of $2t$ with $\tilde{H}_{\mu\nu}$ defined by Eq. (6.109) obeying open boundary conditions are plotted in panels (a-d). Entanglement spectra $\sigma(Q_{\mu\nu A})$ for the equal-time one-point correlation matrix (6.9) derived from $\tilde{H}_{\mu\nu}$ obeying periodic boundary conditions are plotted in panels (f-h). The choices $\delta t = t$ and $V_{\mu\nu} = 0$ for panels (a) and (e), $\delta t = t$ and $V_{12r,rr'} = \delta_{r,r'} (t/10) \chi_{12}$ for panels (b) and (f), $\delta t = t$ and $V_{11r,rr'} = \delta_{r,r'} (t/10) \chi_{11}$ for panels (c) and (g), and $\delta t = 2t/3$ and $V_{13r,rr'} = \delta_{r,r'} (t/10) \chi_{11}$ for panels (d) and (h) are made. The spectra in panels (b) and (f) are unchanged if $V_{12}$ is replaced by either $V_{03}$ or $V_{33}$.

6.4.4 Stability analysis of the zero modes

The topological classification of non-interacting fermionic insulators based on the presence or absence of the discrete symmetries under the operations of time reversal, charge conjugation, and chirality satisfies a bulk-edge (holography) correspondence principle. According to this principle a non-vanishing value for a certain topological index defined for the bulk is equivalent to the existence of extended boundary states on physical boundaries. This correspondence is lost when crystalline symmetries such as inversion about a point or reflection about a mirror plane are also imposed. What remains is a symmetry-protected topological classification of non-interacting bulk fermionic insulators that obey a crystalline symmetry[160, 161]. This classification has two distinctive features. First, a symmetry-protected topologically phase is not required to support extended boundary states localized at the physical edges. Second, a bulk-edge correspondence principle is nevertheless believed to hold for the entanglement spectrum.

We are going to verify how this correspondence principle for symmetry-protected topologically phases of non-interacting fermionic insulating phases holds for the one-dimensional model with the elementary building block defined by Eq. (6.87) and explain why. When $(\mu, \nu) = (0, 0); (1, 1); (2, 1); (3, 0)$, we are going to show that $\tilde{H}_{\mu\nu}$ defined
in Eq. (6.109) fail to support robust edge states for an open geometry, whereas \( \bar{Q}_{\mu\nu A} \) supports robust edge states at the entangling boundaries.

To this end, our strategy is going to be to first explain the rows of Table 6.1. We shall then choose a combination of symmetry under time reversal and spectral symmetry under charge conjugation that puts \( \bar{H}_{\mu\nu} \) in the Cartan symmetry class CI. This symmetry class is a topologically trivial one, a generic perturbation of \( \bar{H}_{\mu\nu} \) destroys any boundary state that \( H_{\mu\nu} \) supports at a physical boundary. However, we shall show that imposing a suitable symmetry under parity guarantees the existence of protected boundary states in the entanglement spectrum \( \sigma(\bar{Q}_{\mu\nu A}) \).

If periodic boundary conditions are imposed, a perturbation that commutes with the parity transformation generated by \( X_{10} \) is of the general form

\[
V_k := \sum_{\nu=0}^{3} \sum_{\mu=0,1} f_{\mu\nu;k} + \sum_{\mu=2,3} g_{\mu\nu;k} \chi_{\mu\nu},
\]

where the functions \( f_{\mu\nu;k} \) and \( g_{\mu\nu;k} \) are even and odd under the inversion \( k \to -k \), respectively [recall Eq. (6.96b)]. For simplicity, the perturbation \( V_k \) is taken independent of \( k \), i.e.,

\[
V_k := \sum_{\nu=0}^{3} \sum_{\mu=0,1} v_{\mu\nu} \chi_{\mu\nu} = \chi_{10} V_{-k} \chi_{10}
\]

with the eight parameters \( v_{\mu\nu} \) real valued. In the orbital basis, we have

\[
V_{r,r'} = \delta_{r,r'} \left[ v_{01} \chi_{01} + v_{02} \chi_{02} + v_{00} \chi_{00} + v_{03} \chi_{03} \right] + \delta_{r,r'} \left[ v_{10} \chi_{10} + v_{11} \chi_{11} + v_{12} \chi_{12} + v_{13} \chi_{13} \right].
\]

The terms that have been underlined twice anti-commute with the two commuting matrices \( \chi_{03} \) and \( \chi_{33} \) that share the zero modes as eigenstates. Hence, the zero modes are protected as a set against the parity-preserving perturbations that are linear combinations of \( \chi_{01} \) and \( \chi_{02} \). All other terms in Eq. (6.108) fail to anti-commute with both \( \chi_{03} \) and \( \chi_{33} \). The zero modes are not necessarily protected as a set under these parity-preserving perturbations. The terms in Eq. (6.108) that are underlined once either anti-commute with \( \chi_{03} \) or \( \chi_{33} \) but not with both. The terms in Eq. (6.108) that are not underlined fail to anti-commute with both \( \chi_{03} \) and \( \chi_{33} \).

The same exercise can be repeated for the parity transformations generated by \( \chi_{01}, \chi_{20}, \) and \( \chi_{31} \). This deliver the first fourteen rows in Table 6.1.
For any $\mu, \nu = 0, 1, 2, 3$, we define the single-particle Hamiltonian $\tilde{H}_{\mu\nu} \equiv H + \mathcal{V}_{\mu\nu}$ by its matrix elements

$$\tilde{H}_{\mu\nu r,r'} := H_{r,r'} + \mathcal{V}_{\mu\nu r,r'},$$

(6.109a)

$$\mathcal{V}_{\mu\nu r,r'} := \delta_{r,r'} v_{\mu\nu} \mathcal{X}_{\mu\nu}.$$  

(6.109b)

The single-particle Hamiltonian $H_{r,r'}$ was defined in Eq. (6.87e) for $r, r' = 1, \ldots, N - 1$. We choose between imposing open boundary conditions by setting the hopping amplitudes to zero between sites $N$ and $N + 1$ or periodic boundary conditions. The perturbation strength $v_{\mu\nu}$ is real-valued. It will be set to $t/10$. The corresponding equal-time one-point correlation matrix defined by Eq. (6.9) is denoted $\tilde{Q}_{\mu\nu}$.

For illustrative purposes, we plot in Figs. 6.3(a-d) the energy eigenvalue spectrum $\sigma(\tilde{H}_{\mu\nu})$ of $\tilde{H}_{\mu\nu}$ obeying open boundary conditions by an exact diagonalization with $N = 12$ that can be extrapolated to the thermodynamic limit. Energy eigenvalues are measured in units of $2t$. In panels (a-c), $\delta t = t$ implies that all energy eigenstates have wavefunctions that are localized on a pair of consecutive sites for which the hopping amplitude is $t + \delta t = 2t$. In the remaining panel (d), a $\delta t \neq t$ delocalizes bulk energy eigenstates that acquire a dispersion, i.e., a band width. The zero modes in panel (a) are four edge states. They are protected by the chiral symmetry in that they are eigenstates of either $\mathcal{X}_{03}$ or $\mathcal{X}_{33}$. For example, they are robust to changing the value of $\delta t$ away from $t$. However, these zero modes are shifted to non-vanishing energies by the perturbations $\mathcal{V}_{12}$ for panel (b) and $\mathcal{V}_{11}$ for panels (c-d). The spectrum in panel (b) is unchanged by the substitutions $\mathcal{V}_{12} \rightarrow \mathcal{V}_{03} \rightarrow \mathcal{V}_{33}$. The presence or absence of protected (against the perturbation from the second column) zero modes localized on the physical boundaries has been verified in this way for all rows and is reported in the penultimate column of Table 6.1.

We plot in Figs. 6.3(e-h) the eigenvalue spectrum $\sigma(\tilde{Q}_{\mu\nu A})$ of the upper-left block $\tilde{Q}_{\mu\nu A}$ in the equal-time one-point correlation matrix $\tilde{Q}_{\mu\nu}$ corresponding to $\tilde{H}_{\mu\nu}$ obeying periodic boundary conditions by an exact diagonalization with $N = 12$ that can be extrapolated to the thermodynamic limit. Panels (e-g) have $\delta t = t$. Panel (h) has $\delta t = 2t/3$. There is no perturbation in panel (e), in which case four zero modes are present in the spectrum $\sigma(\tilde{Q}_{\mu\nu A})$. The perturbation $\mathcal{V}_{12}$ splits the four zero modes into two pairs of degenerate eigenstates with eigenvalues only differing by their sign in panel (f), as was the case for the Hamiltonian in panel (b). The spectrum in panel (f) is unchanged by the substitutions $\mathcal{V}_{12} \rightarrow \mathcal{V}_{03} \rightarrow \mathcal{V}_{33}$. Unlike in panels (c) and (d) for the Hamiltonian, panels (g) and (h) show that the four zero modes of $\tilde{Q}_{\mu\nu A}$ are robust to the perturbation $\mathcal{V}_{11}$.

The lesson from Fig. 6.3 and Table 6.1 is that of all the seven

$$\mathcal{V}_{00}, \mathcal{V}_{03}, \mathcal{V}_{11}, \mathcal{V}_{12}, \mathcal{V}_{21}, \mathcal{V}_{22}, \mathcal{V}_{30}$$

(6.110)
out of fourteen parity-preserving perturbations that gap the zero modes of $\mathcal{H}$, only four, namely

$$V_{00}, V_{11}, V_{21}, V_{30},$$

fail to also gap the zero modes of $Q_A$.

To explain this observation, we rely on the reasoning that delivers Table 6.2. We assume that the underlying microscopic model has the triplet of symmetries $(\mathcal{P}; \mathcal{T}; \mathcal{C}) \sim (\mathcal{P}_{\mu \nu}, \mathcal{T}_{\mu \nu}, \mathcal{C}_{\mu \nu})$ where the doublet $(\mathcal{T}, \mathcal{C}) \sim (\mathcal{T}_{\mu \nu}, \mathcal{C}_{\mu \nu})$ defines the symmetry class CI, i.e., $T_{\mu \nu}^2 = +1$ and $C_{\mu \nu}^2 = -1$. We denote the most general perturbation that is compliant with the triplet of symmetries $(\mathcal{P}; \mathcal{T}; \mathcal{C})$ defining a given row of Table 6.2 by $V_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$. The explicit form of this perturbation is to be found in the second column of Table 6.2 as one varies $(\mathcal{P}; \mathcal{T}; \mathcal{C})$. For a given row in Table 6.2, $V_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ is contained in the most general perturbation $V_{\mathcal{T}; \mathcal{C}}$ that is compliant with the doublet of symmetries $(\mathcal{T}, \mathcal{C})$.

We define the single-particle Hamiltonian $H_{\mathcal{P}; \mathcal{T}; \mathcal{C}} \equiv H + V_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ by its matrix elements

$$H_{\mathcal{P}; \mathcal{T}; \mathcal{C}} r, r' := H_{r, r'} + V_{\mathcal{P}; \mathcal{T}; \mathcal{C}} r, r',$$

$$V_{\mathcal{P}; \mathcal{T}; \mathcal{C}} r, r' := \delta_{r, r'} \sum_{\mu, \nu \in \text{row}} v_{\mu \nu} X_{\mu \nu}.$$ 

The corresponding equal-time one-point correlation matrix is $Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ and its upper-left block is $Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}} A$. The third column in Table 6.2 provides two signs for each row. The first sign $\eta_T$ is positive if $\mathcal{P}$ commutes with $\mathcal{T}$ and negative if $\mathcal{P}$ anti-commutes with $\mathcal{T}$. The second sign $\eta_C$ is positive if $\mathcal{P}$ commutes with $\mathcal{C}$ and negative if $\mathcal{P}$ anti-commutes with $\mathcal{C}$. The information contained with the doublet $(\eta_T, \eta_C)$ is needed to read from Table VI of Ref. [161] the bulk topological index of the single-particle Hamiltonian (6.112). This topological index does not guarantee that $H_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ supports boundary states in an open geometry. In fact, $H_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ does not support boundary states in an open geometry, for the physical boundaries are interchanged under the operation of parity $\mathcal{P}$. On the other hand, $Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}} A$ supports boundary states on the entangling boundaries under the following conditions.

Hamiltonian $H_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ is local by assumption and gaped if periodic boundary conditions are imposed. As explained in Sec. 6.3.2, $Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ and all its four blocks inherit this locality. We have shown with Eq. (6.39) that the upper-left block $Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}} A$ inherits the symmetry $\mathcal{T}$ and the spectral symmetry $\mathcal{C}$ of $H_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$. We have also shown with Eq. (6.46) that the symmetry $\mathcal{P}$ of $H_{\mathcal{P}; \mathcal{T}; \mathcal{C}}$ is turned into a spectral symmetry of $Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}} A$ under $\Gamma_{\mathcal{P}} := C_{\mathcal{P}; \mathcal{T}; \mathcal{C}} AB P_{\mathcal{P}}^A$. The unperturbed upper-left block $Q_A$ has two zero modes per entangling boundary. Because of locality, the perturbation

$$\delta Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}} A := Q_{\mathcal{P}; \mathcal{T}; \mathcal{C}} A - Q_A$$

only mixes the two members of a doublet of boundary states of $Q_A$ on a given entangling boundary. Hence, we may
represent the effect of the perturbation $\delta Q_{\mathcal{P};\mathcal{T};\mathcal{C}}$ by imposing on the Hermitian $2 \times 2$ matrix

$$
\delta Q_{\text{boundary}} := \sum_{\mu=0}^{3} a_\mu \rho_\mu, \quad a_\mu \in \mathbb{R},
$$

(\rho_0 is the unit $2 \times 2$ matrix and $\rho_1, \rho_2, \rho_3$ are the Pauli matrices) the condition imposed by the symmetry $\mathcal{T} \sim \rho_0 K$ and the spectral symmetries $\mathcal{C} \sim \rho_2 K$ and $\Gamma_{\mathcal{P}A}$. The first two symmetries imply that

$$
\delta Q_{\text{boundary}} = a_1 \rho_1 + a_3 \rho_3.
$$

A doublet of zero modes is thus protected if and only if

$$
\Gamma_{\mathcal{P}A} := C_{\mathcal{P};\mathcal{T};\mathcal{C}} \rho_{AB} P^I_{AB} \sim \rho_0,
$$

for $\{\rho_0, \delta Q_{\text{boundary}}\} = 0$ can then only be satisfied if $a_1 = a_3 = 0$. We now show that condition (6.116) is only met for the first three rows of Table 6.2, the only rows from Table 6.2 with $(\eta_{\mathcal{T}}, \eta_{\mathcal{C}}) = (+, -)$, i.e., the only choice for the triplet $(P_{\mu\nu}, T_{\mu\nu}, C_{\mu\nu})$ for which

$$
[\mathcal{P}, \mathcal{T}] = 0, \quad \{\mathcal{P}, \mathcal{C}\} = 0.
$$

To see this, we are going to combine Eq. (6.117) with

$$
[C_{\mathcal{P};\mathcal{T};\mathcal{C}} AB, T_{\mathcal{T}}] = 0, \quad \{C_{\mathcal{P};\mathcal{T};\mathcal{C}} AB, C_{\mathcal{C}}\} = 0,
$$

where $T_{\mathcal{T}}$ and $C_{\mathcal{C}}$ represent the actions of time reversal and charge conjugation on the partition grading of the equal-time one-point correlation matrix. If we use the algebraic identity

$$
[\Gamma_{\mathcal{P}A}, T_{\mathcal{T}}] = C_{\mathcal{P};\mathcal{T};\mathcal{C}} AB \left[ P^I_{AB}, T_{\mathcal{T}} \right] + \left[ C_{\mathcal{P};\mathcal{T};\mathcal{C}} AB, T_{\mathcal{T}} \right] P^I_{AB},
$$

$$
[\Gamma_{\mathcal{P}A}, C_{\mathcal{C}}] = C_{\mathcal{P};\mathcal{T};\mathcal{C}} AB \left\{ P^I_{AB}, C_{\mathcal{C}} \right\} - \left\{ C_{\mathcal{P};\mathcal{T};\mathcal{C}} AB, C_{\mathcal{C}} \right\} P^I_{AB},
$$

Eq. (6.119), when combined with Eqs. (6.118) and (6.117), simplifies to

$$
[\Gamma_{\mathcal{P}A}, T_{\mathcal{T}}] = [\Gamma_{\mathcal{P}A}, C_{\mathcal{C}}] = 0.
$$

Equation (6.120) allows us to deduce that $\Gamma_{\mathcal{P}A}$ must be represented by $\rho_0$ on the two-dimensional Hilbert space
spanned by the boundary states on an entangling boundary,

\[ \Gamma \mathcal{P}_A \sim \rho_0. \] (6.121)

Hence, the only \( \delta Q \) boundary in Eq. (6.115) that anti-commutes with \( \rho_0 \) is \( \delta Q \) boundary = 0, thereby proving the stability of the boundary states on an entangling boundary for the first three rows of Table 6.2.

Figure 6.4: The one-dimensional lattice model is defined by Fig. 6.2 with \( N := N_{\text{tot}} / N_{\text{orb}} = 48 / 4 = 12 \) repeat unit cells with either a torus or a cylindrical geometry. The partition is done by defining \( A (B) \) to be the set of all the orbitals localized to the left (right) of the dash-three-dots (green) line \( RVE \) in Fig. 6.2(a). The equal-time-correlation matrix \( C \) is defined in Eq. (6.6). It is a \( 48 \times 48 \) Hermitian matrix with a \( 24 \times 24 \) Hermitian block defining the matrix \( C_A \), see Eq. (6.10c). The symmetry operation is the parity transformation (reflection) \( \mathcal{P} \) about the dash-three-dots (green) line \( RVE \) in Fig. 6.2(a). It interchanges \( A \) and \( B \) while leaving the entangling boundary \( RVE \) unchanged. Hence, \( \mathcal{P} \) can be represented by the \( 48 \times 48 \) matrix \( P \) with the off-diagonal block structure displayed in Eq. (6.40b). There follows the existence of the \( 24 \times 24 \) matrix \( \Gamma_{\mathcal{P}_A} \) defined in Eq. (6.46d) that anti-commutes with \( Q_A := \mathbb{I} - 2 C_A \). The amplitudes of the matrix elements of \( C_A \) and \( \Gamma_{\mathcal{P}_A} \) are represented by the coloring of the \( 24 \times 24 \) elementary plaquettes of a square lattice. The blue (red) color of a plaquette determines the positive (negative) sign of the matrix element. The lighter the color, the smaller the magnitude with white representing zero. The darker the color, the larger the magnitude with \( \mathcal{P} \) the largest magnitude. A \( 24 \times 1 \) rectangular lattice represents as a column vector an eigenstate of \( Q_A := \mathbb{I} - 2 C_A \). (a) The case of Hamiltonian (6.87c) obeying periodic boundary conditions for \( \delta t = t \). The four entangling zero modes are also plotted. (b) The case of Hamiltonian (6.87c) obeying periodic boundary conditions for \( \delta t = t \) and perturbed by \( 0.05 t X_{11} \). The four entangling zero modes are also plotted. (c) The case of Hamiltonian (6.87c) obeying open boundary conditions for \( \delta t = t \) and perturbed by \( 0.05 t X_{11} \). The two entangling zero modes are also plotted. (d) The case of Hamiltonian (6.87c) obeying periodic boundary conditions for \( \delta t = 9t/11 \) and perturbed by \( 0.05 t X_{11} \). The four entangling zero modes are also plotted. (e) The case of Hamiltonian (6.87c) obeying open boundary conditions for \( \delta t = 9t/11 \) and perturbed by \( 0.05 t X_{11} \). The two entangling zero modes are also plotted.
6.4.5 Numerical verification that $\Gamma_P^A$ is local

For completeness, we verify numerically the prediction from Sec. 6.3.2 that $\Gamma_P^A$ is local in that it does not mix zero modes localized on boundaries separated by a bulk-like distance. To this end, we consider Hamiltonian (6.87c) with or without perturbations for $N_{\text{tot}} = 48$ orbitals (twelve repeat unit cells with four orbitals per repeat unit cell, $N = 12$ and $N_{\text{orb}} = 4$). Plotted in Fig. 6.4 as columnar vectors in the orbital basis are the zero modes $\phi$ that are localized at the entangling boundaries.

When periodic boundary conditions are imposed, there are two entangling boundaries separated by the bulk-like distance of order $N/2 = 6$. Correspondingly, there are two zero modes $\phi_{L1}$ and $\phi_{L2}$ localized on the left entangling boundary and there are two zero modes $\phi_{R1}$ and $\phi_{R2}$ localized on the right entangling boundary. They are represented in Figs. 6.4(a), 6.4(b), and 6.4(d) as columnar vectors in the orbital basis. One verifies that the overlap of any pair of zero modes with one zero mode localized on the left entangling boundary and the other zero mode localized on the right entangling boundary are exponentially suppressed in magnitude by a factor of order $\exp(-br\Delta)$ with $b$ a number or order unity and the separation $r$ of order $N/2 = 6$.

When open boundary conditions are imposed, there are two physical boundaries separated by the bulk-like distance of order $N/2 = 6$, and one entangling boundary a distance of order $N/4 = 3$ away from either physical boundaries. The perturbation $0.05t\mathcal{X}_{11}$ has been added to the Hamiltonian (6.87c). According to Table 6.1, this perturbation gaps the zero modes localized on the physical boundaries. Correspondingly, there are two zero modes $\phi_1$ and $\phi_2$ localized on the entangling boundary represented in Figs. 6.4(c) and 6.4(e) by columnar vectors in the orbital basis.

6.5 Topological insulator protected by one reflection symmetry in two dimensions

6.5.1 Hamiltonian and topological quantum numbers

Our second example is defined by choosing $d = 2$ and $N_{\text{orb}} = 4$ in Eq. (6.2). We represent the action on the orbital degrees of freedom by the $4 \times 4$ matrices defined in Eq. (6.95a). The Brillouin zone (BZ) is two-dimensional and the single-particle Hamiltonian admits the direct-sum decomposition

$$\mathcal{H} = \bigoplus_{k \in \text{BZ}} \mathcal{H}_k,$$

and

$$\mathcal{H}_k := [2t (\cos k_1 + \cos k_2) - \mu] \mathcal{X}_{03} - 2\Delta \sin k_1 \mathcal{X}_{31} - 2\Delta \sin k_2 \mathcal{X}_{02},$$
with the real-valued characteristic energy scales $t$, $\Delta$, and $\mu$.

Hamiltonian $\mathcal{H}$ can be interpreted as the direct sum

$$\mathcal{H}_k = \mathcal{H}_k^+ + \mathcal{H}_k^-$$

of the Bogoliubov-de-Gennes Hamiltonian

$$\mathcal{H}_k^+ \sim [2t (\cos k_1 + \cos k_2) - \mu] \tau_3 - 2\Delta [\sin k_1 \tau_1 + \sin k_2 \tau_2]$$

and the Bogoliubov-de-Gennes Hamiltonian

$$\mathcal{H}_k^- \sim [2t (\cos k_1 + \cos k_2) - \mu] \tau_3 + 2\Delta [\sin k_1 \tau_1 - \sin k_2 \tau_2]$$

describing $p_1 + ip_2$ superconducting order. A gap is present when $|\mu| < 4t$, an assumption that is made throughout in Sec. 6.5.

The bundle of single-particle eigenstates obtained by collecting the lower band from the bundle $\{\mathcal{H}_k^+, \ k \in \text{BZ}\}$ has the opposite non-vanishing Chern number to that of the bundle of single-particle eigenstates obtained by collecting the lower band from the bundle $\{\mathcal{H}_k^-, \ k \in \text{BZ}\}$. The bundle of single-particle eigenstates obtained by collecting the lower band from the bundle $\{\mathcal{H}_k, \ k \in \text{BZ}\}$ is topologically trivial.

### 6.5.2 Symmetries

The symmetries of the single-particle Hamiltonian defined by Eq. (6.122) are the following.

1. There are two symmetries of the inversion type. If $\mathcal{I}$ denotes the inversion of space $\mathcal{I}: r \mapsto -r$,

$$\mathcal{I} : r \mapsto -r,$$

then

$$\mathcal{O}_m^{\mathcal{I}} \mathcal{H}_k \mathcal{O}_m = \mathcal{H}_{-k}$$

with

$$\mathcal{O}_m \in \{\mathcal{X}_0, \mathcal{X}_3\}.$$
reflection

\[ \mathcal{R}_1 : r_1 \mapsto +r_1, \quad \mathcal{R}_1 : r_2 \mapsto -r_2, \]  

(6.125a)

then

\[ \mathcal{O}_{\mathcal{R}_1}^I \mathcal{H}_{+k_1,-k_2} \mathcal{O}_{\mathcal{R}_1} = \mathcal{H}_{+k} \]  

(6.125b)

with

\[ \mathcal{O}_{\mathcal{R}_1} \in \{ \mathcal{X}_{13}, \mathcal{X}_{23} \}. \]  

(6.125c)

[3] There are two symmetries of the reflection about the vertical axis \( k = (0, k_2) \) type. If \( \mathcal{R}_2 \) denotes the reflection

\[ \mathcal{R}_2 : r_1 \mapsto -r_1, \quad \mathcal{R}_2 : r_2 \mapsto +r_2, \]  

(6.126a)

then

\[ \mathcal{O}_{\mathcal{R}_2}^I \mathcal{H}_{-k_1,+k_2} \mathcal{O}_{\mathcal{R}_2} = \mathcal{H}_{+k} \]  

(6.126b)

with

\[ \mathcal{O}_{\mathcal{R}_2} \in \{ \mathcal{X}_{10}, \mathcal{X}_{20} \}. \]  

(6.126c)

[4] There are two symmetries of the time-reversal type. If \( \mathcal{T} \) denotes the reversal of time

\[ \mathcal{T} : t \mapsto -t, \]  

(6.127a)

then

\[ \mathcal{O}_{\mathcal{T}}^I \mathcal{H}_{-k} \mathcal{O}_{\mathcal{T}} = \mathcal{H}_{+k} \]  

(6.127b)

with

\[ \mathcal{O}_{\mathcal{T}} \in \{ \mathcal{X}_{10}, \mathcal{X}_{20} \}. \]  

(6.127c)

[5] There are two spectral symmetries of the charge-conjugation type,

\[ \mathcal{O}_{\mathcal{C}}^I \mathcal{H}_{-k}^T \mathcal{O}_{\mathcal{C}} = -\mathcal{H}_{+k} \]  

(6.128a)

with

\[ \mathcal{O}_{\mathcal{C}} \in \{ \mathcal{X}_{01}, \mathcal{X}_{31} \}. \]  

(6.128b)
[6] There are two spectral symmetries of the chiral type,

\[ \mathcal{O} \mathcal{H} \mathcal{O} = -\mathcal{H} \]

with

\[ \mathcal{O} \in \{ X_{11}, X_{21} \}. \]

### 6.5.3 Partition and zero modes

From now on, we adopt a cylindrical geometry instead of the torus geometry from Sec. 6.5.1, i.e., we compactify two-dimensional space \( \{ x := (x_1, x_2) \in \mathbb{R}^2 \} \) only along one Cartesian coordinate. Consequently, only one component of the two-dimensional momentum \( \{ k := (k_1, k_2) \in \mathbb{R}^2 \} \) is chosen to be a good quantum number in Eq. (6.122).

For any choice of the direction \( i = 1, 2 \) along which periodic boundary conditions are imposed while open boundary conditions are imposed along the orthogonal direction \( i + 1 \) modulo 2, for any positive integer \( M_i \), and for any...
good momentum quantum number

\[ k_i = \frac{2\pi}{2M_i a} n_i, \quad n_i = 1, \cdots, 2M_i, \quad i = 1, 2, \]  

(6.130a)

we do the following. First, we denote by \( \mathcal{H}_{k_i} \) the \( 8M_{i+1} \times 8M_{i+1} \) Hermitian matrix such that the one-dimensional Fourier transform of

\[ \mathcal{H}_{k_i} r_{i+1}, r'_{i+1} := \langle r_{i+1} | \mathcal{H}_{k_i} | r'_{i+1} \rangle, \]  

(6.130b)

delivers Eq. (6.122b). Here,

\[ r_{i+1} = n_{i+1} a, \quad n_{i+1} = 1, \cdots, 2M_{i+1}, \]  

(6.130c)

and

\[ r'_{i+1} = n'_{i+1} a, \quad n'_{i+1} = 1, \cdots, 2M_{i+1}, \]  

(6.130d)

are the lattice sites from an open chain along the direction \( i + 1 \) (defined modulo 2) of a rectangular lattice with the lattice spacing \( a \) and the number of lattice sites \( M_{i+1} \) along the direction \( i + 1 \) modulo 2. Second, we define the \( k_i \)-dependent partition

\[ \mathfrak{F} := \bigoplus_{k_i} \mathfrak{F}_{k_i}, \mathfrak{F}_{k_i} := \mathfrak{F}_{A_{i+1}} \oplus \mathfrak{F}_{B_{i+1}}, \]  

(6.131a)

where

\[ \mathfrak{F}_{A_{i+1}} := \bigoplus_{n_{i+1} = 1}^{M_{i+1}} \bigoplus_{\alpha = 1}^{4} \langle k_i, n_{i+1}, \alpha \rangle \langle k_i, n_{i+1}, \alpha \rangle, \]  

(6.131b)

\[ \mathfrak{F}_{B_{i+1}} := \bigoplus_{n_{i+1} = M_{i+1} + 1}^{2M_{i+1}} \bigoplus_{\alpha = 1}^{4} \langle k_i, n_{i+1}, \alpha \rangle \langle k_i, n_{i+1}, \alpha \rangle, \]  

(6.131c)

and the ket \( | k_i, n_{i+1}, \alpha \rangle \) denotes the single-particle state with the Bloch index \( k_i \), for it is extended along the \( i = 1, 2 \) direction, the unit repeat cell index \( n_{i+1} \), for it is localized at the site \( n_{i+1} a \) along the \( i + 1 \) modulo 2 direction, and the orbital index \( \alpha = 1, 2, 3, 4 \). If we denote by \( R_i \) the reflection that leaves \( k_i \) unchanged but reverses the sign of \( k_{i+1} \), i.e.,

\[ R_i k_i = +k_i, \quad R_i k_{i+1} = -k_{i+1}, \]  

(6.132)
we then have that

\[ R_i A_{i+1} = B_{i+1}, \quad R_i B_{i+1} = A_{i+1}, \quad (6.133a) \]
\[ C A_{i+1} = A_{i+1}, \quad C B_{i+1} = B_{i+1}, \quad (6.133b) \]
\[ F A_{i+1} = A_{i+1}, \quad F B_{i+1} = B_{i+1}, \quad (6.133c) \]
\[ S A_{i+1} = A_{i+1}, \quad S B_{i+1} = B_{i+1}. \quad (6.133d) \]

The thermodynamic limit is defined by

\[ N, N_f \rightarrow \infty, \quad (6.134a) \]

with \( N = (2M_1) \times (2M_2) \), holding the fermion density

\[ N_f/N = 1 \quad (6.134b) \]

fixed. In the thermodynamic limit, the single-particle energy eigenvalue spectrum \( \sigma(\mathcal{H}_i) \) of

\[ \mathcal{H}_i := \bigoplus_{k_i} \mathcal{H}_{k_i} \quad (6.135a) \]

supports two pairs of zero modes, each of which are localized at the opposite (physical) boundaries on the cylinder whose symmetry axis coincides with the direction \( i + 1 \) (defined modulo 2) along which open boundary conditions have been imposed. Similarly, the entanglement spectrum \( \sigma(Q_{A_{i+1}}) \) of the equal-time one-point correlation matrix

\[ Q_{A_{i+1}} := I - 2C_{A_{i+1}} \quad (6.135b) \]

supports a pair of zero modes localized at the entangling boundary.

In order not to confuse gapless boundary modes originating from the physical boundaries with gapless boundary modes originating from the entangling boundary, whenever the physical boundaries support gapless boundary states in the energy spectrum, we opt for a torus geometry when computing the entanglement spectrum.

Desired is a study of the stability of these zero modes under all generic perturbations of \( \mathcal{H}_i \) that respect any one \( (\mathcal{S}) \) of the two chiral symmetry from Eq. (6.129) and any one \( (\mathcal{R}) \) of the four reflection symmetries from Eqs. (6.125) and (6.126).
Table 6.3: The spectrum \( \sigma(\tilde{H}_{k_i \mu \nu}) \) of the single-particle Hamiltonian \( \tilde{H}_{k_i \mu \nu} \) defined by Eq. (6.136) and obeying periodic boundary conditions along the \( i = 1, 2 \) direction and open boundary conditions along the \( i + 1 \) (modulo 2) direction. The entanglement spectrum \( \sigma(\tilde{Q}_{k_i \mu \nu A_{i+1}}) \) defined by Eq. (6.12) for the single-particle Hamiltonian \( \tilde{H}_{k_i \mu \nu} \) obeying periodic boundary conditions along both the \( i = 1, 2 \) and the \( i + 1 \) (modulo 2) direction. The entry \( \circ \) or \( \times \) in the second to sixth columns denotes the presence or the absence, respectively, of the symmetries under reflections about the directions 1 (\( R_1 \)) and 2 (\( R_2 \)), charge conjugation \( C \), time reversal \( T \), and chiral \( S \) of the perturbation \( \delta r_{i+1} r_{i+1}^{t} \). The entry \( \otimes \) in the last two columns denotes the existence of crossings between the mid-gap branches, whereby the crossings are away from vanishing energy (entanglement eigenvalue) and vanishing momentum in the spectra \( \sigma(\tilde{H}_{k_i \mu \nu}) \) and \( \sigma(\tilde{Q}_{k_i \mu \nu A_{i+1}}) \) as determined by extrapolation to the thermodynamic limit of exact diagonalization with the open direction running over 32 repeat unit cells and the momentum along the compactified direction running over 128 values. The entry \( \otimes \) in the last two columns denotes the existence of crossings between the mid-gap branches, whereby the crossings are away from vanishing energy (entanglement eigenvalue) and vanishing momentum in the spectra \( \sigma(\tilde{H}_{k_i \mu \nu}) \) and \( \sigma(\tilde{Q}_{k_i \mu \nu A_{i+1}}) \).
6.5.4 Stability analysis of the zero modes

Definitions of $\tilde{H}_{i\mu\nu}$ and $\tilde{Q}_{k_i\mu\nu A_{i+1}}$

To begin with the stability analysis, we choose $i = 1, 2$ and perturb Hamiltonian (6.130b) by adding locally any one of the sixteen matrices $X_{\mu\nu} \equiv \sigma_{\mu} \otimes \tau_{\nu}$ parametrized by $\mu, \nu = 0, 1, 2, 3$. Thus, we define

$$\tilde{H}_{i\mu\nu} := \bigoplus_{k_i} \tilde{H}_{k_i\mu\nu} \equiv \bigoplus_{k_i} \left( H_{k_i} + V_{\mu\nu} \right) \quad (6.136a)$$

by the matrix elements

$$\tilde{H}_{k_i\mu\nu r_{i+1}, r'_{i+1}} := H_{k_i r_{i+1}, r'_{i+1}} + V_{\mu\nu r_{i+1}, r'_{i+1}} \quad (6.136b)$$

$$V_{\mu\nu r_{i+1}, r'_{i+1}} := \delta_{r_{i+1}, r'_{i+1}} v_{\mu\nu} X_{\mu\nu} \quad (6.136c)$$

where the matrix elements of $H_{k_i}$ were defined in Eq. (6.130) and the perturbation strength $v_{\mu\nu}$ is real valued.

Equipped with $\tilde{H}_{k_i\mu\nu}$, we define $\tilde{Q}_{k_i\mu\nu A_{i+1}}$ from Eq. (6.12) with the caveat that periodic boundary conditions are imposed along the direction $i + 1$ (modulo 2).

Spectra $\sigma(\tilde{H}_{i\mu\nu})$

For any $i = 1, 2$, the spectra $\sigma(\tilde{H}_{i\mu\nu})$ for $\mu, \nu = 0, 1, 2, 3$ were obtained from exact diagonalization with the unperturbed energy scales $t = \Delta = -\mu = 1$. These spectra are characterized by two continua of single-particle excitations separated by an energy gap as is illustrated in Figs. 6.5(a-d). A discrete number (four) of branches are seen to peel off from these continua, some of which eventually cross the band gap. These mid-gap branches disperse along the physical boundaries (edges) while they decay exponentially fast away from the edges. They are thus called edge states. Their crossings, if any, define degenerate edge states with group velocities of opposite signs along the edges. Their crossings at vanishing energy and momentum, if any, define degenerate non-propagating zero modes with group velocities of opposite signs along the edges. Their crossings at vanishing energy and non-vanishing momenta, if any, define degenerate propagating zero modes with group velocities of opposite signs along the edges. Their crossings at non-vanishing energies and vanishing momentum, if any, define degenerate non-propagating edge states with group velocities of opposite signs along the edges. The entries ○ in the last two columns of Table 6.3 accounts for the existence of at least one crossing at vanishing energy and momentum. The entries ⊗ in the last two columns of Table 6.3 account for the existence of crossings not necessarily at vanishing energy and momentum. The entries × in the last two column of Table 6.3 accounts for the absence of crossings.
The origin of the mid-gap branches in Figs. 6.5(a-f) is the following. The single-particle Hamiltonian defined in Eq. (6.122b) for a torus geometry supports four boundary states for a cylindrical geometry that are extended along the boundary but exponentially localized away from the boundary due to the non-vanishing Chern numbers for each of $H_k^+$ and $H_k^-$. These dispersing boundary states show up in the single-particle energy spectrum as four branches of mid-gap states that cross at vanishing energy and momentum, thereby defining four degenerate non-propagating zero modes. In the presence of the perturbation $0.3 \; t \; \mathcal{X}_{13}$ when the boundary dictates that $k_1$ is a good quantum number, the energy spectrum shows a four-fold degenerate crossing at vanishing energy and momentum in Fig. 6.5(a). However, the very same perturbation, when the boundary dictates that $k_2$ is a good quantum number, gaps the unperturbed crossing at vanishing energy and momentum in Fig. 6.5(b). In the presence of the perturbation $0.3 \; t \; \mathcal{X}_{02}$ when the boundary dictates that $k_2$ is a good quantum number, the energy spectrum shows a four-fold-degenerate crossing at vanishing energy but away from $k_2 = 0$ in Fig. 6.5(c). In the presence of the perturbation $0.3 \; t \; \mathcal{X}_{32}$ when the boundary dictates that $k_2$ is a good quantum number, the energy spectrum shows four non-degenerate crossings away from vanishing energy and vanishing momentum in Fig. 6.5(d). Even though all the crossings in the unperturbed entanglement spectra are robust to the perturbations in Fig. 6.5(e-h), they can be shifted away from vanishing energy as in Fig. 6.5(h) or momentum as in Fig. 6.5(g).

To understand the effect of any one of the sixteen perturbations from Table 6.3 on the zero modes of Hamiltonian $\mathcal{H}_i$ defined in Eq. (6.135a), where $i = 1, 2$ is the choice made along the direction for which periodic boundary conditions is imposed [recall Eq. (6.130)], it is useful to consider Fig. 6.6. The physical boundaries are the two circles centered at $L$ and $R$ on the symmetry axis $i + 1$ modulo 2 of the cylinder in Fig. 6.6. In the limit for which the band gap is taken to infinity, the effective theory for the single-particle eigenstates of $\mathcal{H}_i$ defined in Eq. (6.135a) that are propagating along the edges $L$ and $R$ with the same group velocity but localized away from them takes the form

$$\mathcal{H}_{\text{edges}} k_i = k_i Y_{33} \quad i = 1, 2. \tag{6.137a}$$

Here, we have set the group velocity to unity and

$$Y_{\mu\nu} := \rho_{\mu} \otimes \varrho_{\nu}, \tag{6.137b}$$

where we have introduced the two sets of unit $2 \times 2$ matrix and Pauli matrices $\rho_{\mu}$ with $\mu = 0, 1, 2, 3$ and $\varrho_{\nu}$ with $\nu = 0, 1, 2, 3$. The eigenvalue $-1$ of $\varrho_3$ is interpreted as the left edge $L$ in Fig. 6.6. The eigenvalue $+1$ of $\varrho_3$ is interpreted as the right edge $R$ in Fig. 6.6. Hence, The matrices $\varrho_1$ and $\varrho_2$ mix edge states localized on opposite edges. The eigenstates of $\rho_3$ describe right and left movers on a given edge. The matrices $\rho_1$ and $\rho_2$ mix left and right movers on a given edge. Hamiltonian (6.137) describes four single-particle states propagating along the two edges...
with the momentum $\pm k_i$. These single-particle states are solely supported on the edges, reason for which we call them edge states. Their direction of propagation originates from the relative sign in $p_1 \pm ip_2$ if $H_i$ is interpreted as a Bogoliubov-de-Gennes superconductor.

A generic perturbation to the effective Hamiltonian (6.137) that allows mixing between all four edge states is

$$
V_{\text{edges}} = \sum_{\mu, \nu = 0}^{3} v_{\text{edges} \mu \nu} Y_{\mu \nu}, \quad v_{\text{edges} \mu \nu} \in \mathbb{R},
$$

(6.138)

to lowest order in a gradient expansion. For any given $\mu, \nu = 0, 1, 2, 3$, the perturbation

$$
V_{\text{edges} \mu \nu} := v_{\text{edges} \mu \nu} Y_{\mu \nu}
$$

(6.139)

opens a gap in the spectrum of

$$
\tilde{H}_{\text{edges} k_{i \mu \nu}} := H_{\text{edges} k_{i \mu \nu}} + V_{\text{edges} \mu \nu}
$$

(6.140)

if it anti-commutes with $Y_{33}$, thereby forbidding the crossing of the bulk gap by any one of the four mid-gap branches from the effective Hamiltonian (6.137). This is what happens in Fig. 6.5(b). A perturbation $V_{\text{edges} \mu \nu}$ that commutes with $Y_{33}$ can shift the location of the two crossings of the four mid-gap branches from the effective Hamiltonian (6.137) away from either vanishing energy or vanishing momentum. For example, the perturbation $V_{\text{edges} 33}$ with $v_{\text{edges} 33} < 0$ moves the crossing in the effective Hamiltonian (6.137) to the right, as happens in Fig 6.5(c). Figure 6.5(d) is realized when only one of $v_{\text{edges} 03}$ and $v_{\text{edges} 30}$ are non-vanishing in the perturbation (6.139). Evidently, Fig 6.5(a) suggests that not all perturbations parametrized by (6.138) move the degenerate crossing of the effective Hamiltonian Eq. (6.137).

To understand Fig 6.5(a), we assume that the perturbation $V_{\text{edges}}$ is local and that the ratio $\xi/L$, where $L$ is the length of the cylinder while $\xi \propto 1/\Delta$ is the bulk correlation length associated to the bulk gap $\Delta$, is taken to zero. Hence, the effective edge theory for

$$
\tilde{H}_{k_{i \mu \nu}} := \tilde{H}_{k_{i \mu \nu}} + V_{\mu \nu}
$$

(6.141)

remains block diagonal, with one of the block given by

$$
\tilde{H}_{\text{edge} k_{i}} = v_0 \rho_0 + v_1 \rho_1 + v_2 \rho_2 + (k_i + v_3) \rho_3
$$

(6.142a)

for some effective real-valued couplings $v_0, v_1, v_2,$ and $v_3$. As was the case for the bulk Hamiltonian (6.122),

$$
\tilde{H}_{\text{edge} k_{i}} := k_i \rho_3 =: \tilde{H}_{\text{edge} k_{i \mu \nu}} - \vec{V}_{\text{edge} \mu \nu}
$$

(6.142b)
obeys two spectral chiral symmetries, for it anti-commutes with $\rho_1$ and $\rho_2$. Moreover, $H_{\text{edge}}k_i$ commutes with the operation by which $k_i \rightarrow -k_i$ is composed with the conjugation of $H_{\text{edge}}k_i$ with either $\rho_1$ and $\rho_2$. Imposing simultaneously this pair of chiral symmetries and this pair of reflection symmetries restricts the effective edge theory to Eq. (6.142b). However, these symmetry constraints are redundant to enforce the form (6.142b) as we now show.

The crossing at vanishing energy and momentum of Hamiltonian (6.142b) is not generically robust to the perturbations in the perturbed Hamiltonian (6.142a). However, if we impose that the perturbed Hamiltonian (6.142a) anti-commutes with either $\rho_1$ or $\rho_2$, i.e., the effective perturbed Hamiltonian belongs to the symmetry class AIII, then the edge theory simplifies to the direct sum over blocks of the form

$$H_{\text{edge}}^{\text{AIII}}k_i \mu \nu = v_2 \rho_2 + (k_i + v_3) \rho_3.$$  

Here, we have chosen, without loss of generality, to implement the chiral symmetry by demanding that $H_{\text{edge}}^{\text{AIII}}k_i \mu \nu$ anti-commutes with $\rho_1$. As is, the perturbations in Hamiltonian (6.143) still gaps the unperturbed dispersion (6.142b). However, if we impose the symmetry constraint

$$\rho_1 H_{\text{edge}}(-k_i) \mu \nu \mathcal{R} \rho_1 = H_{\text{edge}}(+k_i) \mu \nu \mathcal{R}$$  

(6.144)

to define $H_{\text{edge}}k_i \mu \nu \mathcal{R}$, we find that

$$H_{\text{edge}}k_i \mu \nu \mathcal{R} = k_i \rho_3.$$  

(6.145)

In other words, if we impose, in addition to the chiral symmetry, the reflection symmetry generated by $\rho_1$ and $k_i \rightarrow -k_i$, we find that no perturbation can gap the unperturbed dispersion (6.142b). Had we chosen to impose the reflection symmetry generated by $\rho_2$ instead of $\rho_1$, i.e., a realization of parity that anti-commutes with the choice $\rho_1$ we made to implement the chiral transformation, then the perturbation $v_2 \rho_2$ in Eq. (6.143) would not be prevented from removing the crossing of the edge states through a spectral gap.

Now, the reflection symmetry obeyed by the effective edge Hamiltonian (6.142b) can only originate from a reflection about the plane frame in blue that contains the cylinder axis in Fig. 6.6. A reflection about the plane framed in red that is orthogonal to the cylinder axis in Fig. 6.6 exchanges the edges $L$ and $R$. As such, it can only be represented within the representation defined by Eqs. (6.137) and (6.138) of the effective edge Hamiltonian that allows mixing of the two opposite edges.
Figure 6.6: A cylinder of length $L$ along the $i + 1$ modulo 2 direction, while the coordinate $i = 1, 2$ has been compactified. We define two reflection planes. The first is defined by the blue frame that includes the cylinder axis. The second is defined by the red frame normal to the cylinder axis and intersecting the cylinder axis at its mid-point. The circles centered at the point L and R on the cylinder axis are the two disconnected boundaries of the cylinder. The reflection about the plane framed in blue leaves each circle invariant as a set. The reflection about the plane framed in red exchanges the circles centered on the cylinder axis at L and R. This plane framed in red defines the entangling boundary in a cylindrical geometry as defined by the partition (6.131).

Spectra $\sigma(\tilde{Q}_{\mu\nu A, i+1})$

For any $i = 1, 2$, the spectra $\sigma(\tilde{Q}_{\mu\nu A, i+1})$ for $\mu, \nu = 0, 1, 2, 3$ were also obtained from exact diagonalization with the unperturbed energy scales $t = \Delta = -\mu = 1$. These spectra are characterized by two nearly flat bands at $\pm 1$ from which pairs of mid-gap branches occasionally peel off as is illustrated in Figs. (6.5) (e-f). We observe in both Figs. (6.5) (e) and (6.5) (f) one crossing of the mid-gap branches at vanishing entanglement eigenvalue and momentum. The crossing in (6.5) (g) takes place at vanishing entanglement eigenvalue but non-vanishing momentum. The crossing in (6.5) (h) takes place at non-vanishing entanglement but vanishing momentum. Crossings of the mid-gap branches taking place at vanishing entanglement eigenvalue and momentum are indicated by $\circ$ in the last two columns of Table 6.3. The absence of any crossing of the mid-gap branches is indicated by $\times$ in the last two columns of Table 6.3. Crossings of the mid-gap branches taking place away from vanishing entanglement eigenvalue and momentum are indicated by $\otimes$ in the last two columns of Table 6.3.

Comparison of Figs. (6.5) (a-d) and Figs. (6.5) (e-f) suggests that the existence of crossings in the entanglement spectrum defined by Eq. (6.135b) is more robust to perturbations than that for the Hamiltonian spectrum. Choose $i = 1, 2$ ($i + 1$ modulo 2), $\mu = 0, 1, 2, 3$, and $\nu = 0, 1, 2, 3$. According to Table 6.3 any crossing in the perturbed Hamiltonian spectrum $\sigma(\tilde{H}_{i, \mu\nu})$ implies a crossing in the perturbed entanglement spectrum $\sigma(\tilde{Q}_{\mu\nu A, i+1})$. The converse is not true. There are crossings in the perturbed entanglement spectrum $\sigma(\tilde{Q}_{\mu\nu A, i+1})$ but no crossings in the perturbed Hamiltonian spectrum $\sigma(\tilde{H}_{i, \mu\nu})$, as is shown explicitly when comparing Fig. (6.5) (f) to Fig. (6.5) (b). In fact, Table 6.3 shows the following difference between the perturbed Hamiltonian and entanglement spectra. On the one hand, the existence of
crossings in \( \sigma(\tilde{H}_{i\mu\nu}) \) does not necessarily imply the existence of crossings in \( \sigma(\tilde{H}_{(i+1)\mu\nu}) \). On the one hand, the existence of crossings in \( \sigma(\tilde{Q}_{\mu\nu A_{i+1}}) \) implies the existence of crossings in \( \sigma(\tilde{Q}_{\mu\nu A_{i+1}}) \) and vice versa.

To understand the effect of any one of the sixteen perturbations from Table 6.3 on the zero modes of \( Q_{A_{i+1}} \) defined in Eq. (6.135b), where \( i + 1 \mod 2 \) is the choice made for the direction along which the partition is made [recall Eq. (6.130)], it is useful to consider the compactification along the cylinder axis of Fig. 6.6 consisting in identifying the circles at L and R. We thereby obtain a torus, whose intersection with the plane framed in red from Fig. 6.6 defines two entangling boundaries separated by the distance \( L/2 \). The spectrum \( \sigma(Q_{A_{i+1}}) \) supports four mid-gap branches, two per entangling boundary. In the limit for which the band gap is taken to infinity, the effective theory for the eigenstates of \( Q_{A_{i+1}} \) that propagate along the entangling boundaries but are localized away from them is given by

\[
Q_{\text{edges}} k i A_{i+1} = k i Y_{33}. \tag{6.146}
\]

The interpretation of the \( 4 \times 4 \) matrices \( Y_{\mu\nu} \) with \( \mu, \nu = 0, 1, 2, 3 \) is the same as the one given below Eq. (6.137b).

A generic perturbation to the effective Hamiltonian (6.146) that allows mixing between all four entangling states is

\[
\delta Q_{\text{edges}} A_{i+1} = \sum_{\mu, \nu = 0}^3 v_{\text{edges}} \mu\nu A_{i+1} Y_{\mu\nu}, \quad v_{\text{edges}} \mu\nu A_{i+1} \in \mathbb{R}, \tag{6.147}
\]

to lowest order in a gradient expansion. For any given \( \mu, \nu = 0, 1, 2, 3 \), the perturbation

\[
\delta Q_{\text{edges}} \mu\nu A_{i+1} := v_{\text{edges}} \mu\nu A_{i+1} Y_{\mu\nu} \tag{6.148}
\]

opens a gap in the spectrum of

\[
\tilde{Q}_{\text{edges}} k_i \mu\nu A_{i+1} := Q_{\text{edges}} k_i A_{i+1} + \delta Q_{\text{edges}} \mu\nu A_{i+1} \tag{6.149}
\]

if it anti-commutes with \( Y_{33} \), thereby forbidding the crossing of the bulk gap by any one of the four mid-gap branches from the effective Hamiltonian (6.146). A perturbation \( V_{\text{edges}} \mu\nu A_{i+1} \) that commutes with \( Y_{33} \) can shift the location of the two crossings of the four mid-gap branches from the effective Hamiltonian (6.146) away from either vanishing energy or vanishing momentum.

To understand the robustness of the effective (6.146) to perturbations, we assume that the perturbation \( V_{\text{edges}} A_{i+1} \) is local and that the ratio \( \xi/L \), where \( L \) is the length of the cylinder while \( \xi \propto 1/\Delta \) is the bulk correlation length associated to the bulk gap \( \Delta \), is taken to zero. Hence, the effective edge theory for

\[
\tilde{Q}_{\mu\nu A_{i+1}} := Q_{A_{i+1}} + \delta Q_{\mu\nu A_{i+1}} \tag{6.150}
\]
remains block diagonal, with one of the block given by

$$\tilde{Q}_{\text{edge} k_i A_{i+1}} = v_0 \rho_0 + v_1 \rho_1 + v_2 \rho_2 + (k_i + v_3) \rho_3 \quad (6.151)$$

for some effective real-valued couplings $v_0$, $v_1$, $v_2$, and $v_3$.

To proceed, we recall that if $S$ is a unitary spectral symmetry of $\mathcal{H}$ in that $S^{-1} \mathcal{H} S = -\mathcal{H}$ and if $S$ is block diagonal with respect to the partition into $A$ and $B$, we then deduce from

$$Q = S^{-1} (-1) QS \quad (6.152)$$

that

$$S_A^{-1} Q_A S_A = -Q_A, \quad S_B^{-1} Q_B S_B = -Q_B. \quad (6.153a)$$

and

$$S_A^{-1} C_{AB} S_B = -C_{AB}, \quad S_B^{-1} C_{BA} S_A = -C_{BA} \quad (6.153b)$$

As was the case for the bulk Hamiltonian $\mathcal{H}$,

$$\tilde{Q}_{\text{edge} k_i A_{i+1}} := k_i \rho_3 \quad (6.154)$$

obeys two spectral chiral symmetries, for it anti-commutes with $\rho_1$ and $\rho_2$, and two spectral symmetries under charge conjugation, for it anti-commutes with the composition of $k_i \rightarrow -k_i$ with conjugation by $\rho_0$ or $\rho_3$.

The crossing at vanishing energy in Eq. (6.154) is not generically robust to the perturbations in Eq. (6.151). However, if we impose that Eq. (6.151) anti-commutes with either $\rho_1$ or $\rho_2$, then the entangling theory simplifies to the direct sum over blocks of the form

$$Q_{\text{edge} k_i \mu \nu A_{i+1}}^{AIII} = v_2 \rho_2 + (k_i + v_3) \rho_3. \quad (6.155)$$

Here and without loss of generality, we have chosen to implement the chiral symmetry by demanding that $Q_{\text{edge} k_i \mu \nu A_{i+1}}^{AIII}$ anti-commutes with $\rho_1$. As is, one perturbation in Hamiltonian $\mathcal{H}$ still gaps the unperturbed dispersion (6.154). However, if we impose the symmetry constraint

$$\rho_2 \tilde{Q}_{\text{edge} k_i \mu \nu A_{i+1}}^{\mathcal{R}_i} \rho_2 = \tilde{Q}_{\text{edge} k_i \mu \nu A_{i+1}}^{\mathcal{R}_i} \quad (6.156)$$
to define \( \tilde{Q}_{\text{edge}} k_i \mu \nu A_{i+1} \mathcal{A}_i \), we find that

\[
\tilde{Q}_{\text{edge}} k_i \mu \nu A_{i+1} \mathcal{A}_i = (k_i + v_3) \rho_3
\]  

(6.157)

displays a crossing at vanishing energy and momentum \( k_i = -v_3 \). In other words, if we impose, in addition to the chiral symmetry, the effective chiral symmetry generated by \( \rho_2 \), we find that no perturbation can gap the unperturbed dispersion (6.154), although it can move the momentum of the zero mode away from vanishing energy. As is implied by the notation, the effective chiral symmetry generated by \( \rho_2 \) originates from protecting the symmetry class AIII by demanding that reflection symmetry about the plane defining the entangling boundaries, i.e., the plane framed in red in Fig. 6.6 holds. According to Sec. 6.3.2, the reflection about the plane framed in red in Fig. 6.6 induces a local effective chiral symmetry of the form given in Eq. (6.46), i.e., there exists a

\[
\Gamma_{\mathcal{A}_i} := C A_{i+1} B_{i+1} k_i R_i
\]  

(6.158)

such that

\[
\left\{ \Gamma_{\mathcal{A}_i}, \tilde{Q}_{\text{edge}} k_i \mu \nu A_{i+1} \mathcal{A}_i \right\} = 0.
\]  

(6.159)

The choice to represent \( \Gamma_{\mathcal{A}_i} \) by \( \rho_2 \), given the choice to represent the chiral symmetry \( \mathcal{S} \) by \( \rho_1 \), is a consequence of the following assumption and the following fact. First, we demand that \( \mathcal{S} \) and \( \mathcal{R}_i \) commute, i.e., we demand that

\[
[S, \mathcal{R}_i] = 0.
\]  

(6.160)

Second, the identity

\[
\left\{ S, \mathcal{R}_i \right\} = \left\{ S, C A_{i+1} B_{i+1} k_i \mathcal{R}_i \right\}
\]

\[
= \left\{ S, C A_{i+1} B_{i+1} k_i \right\} \mathcal{R}_i - C A_{i+1} B_{i+1} k_i \left[ S, \mathcal{R}_i \right]
\]  

(6.161)

holds.

**Spectra** \( \sigma(\mathcal{H}_k, \mathcal{A}; \mathcal{S}) \) and \( \sigma(Q_k, \mathcal{A}; \mathcal{S}_{A_{i+1}}) \)

It is time to present the reasoning that delivers Table 6.4. Let \( i = 1, 2 \) and define \( i + 1 \) modulo 2. We assume that the underlying microscopic model has the doublet of symmetries \( (\mathcal{A}; \mathcal{S}) \sim (\mathcal{R}_{\mu \nu}, \mathcal{S}_{\mu \nu}) \) where \( \mathcal{S} \sim \mathcal{S}_{\mu \nu} \) defines the symmetry class AIII. We denote the most general perturbation that is compliant with the doublet of symmetries \( (\mathcal{A}; \mathcal{S}) \) defining a given row of Table 6.2 by \( \mathcal{V}_{\mathcal{A}; \mathcal{S}} \). The explicit form of this perturbation is to be found in the second
Table 6.4: The first four rows of the second column give all possible doublets of generators consisting of a reflection about the direction 1 and a chiral transformation. The last four rows of the second column give all possible doublets of generators consisting of a reflection about the direction 2 and a chiral transformation. The third column gives for each row the most general perturbation $V_{\phi,\phi}$ that commutes with the operation of reflection and anti-commutes with the operation of chirality. The fourth column gives the sign $\eta_\phi$ defined by $R S R = \eta_\phi S$. The fifth column is an application of the classification for the symmetry-protected topological band insulators in two-dimensional spaces derived in Refs. [160] and [161] (Table VI from Ref. [161] was particularly useful). The topological indices $Z$ and $0$ correspond to topologically nontrivial and trivial bulk phases, respectively. The entries $\circ$ or $\times$ in the last two columns denote the presence or absence, respectively, of zero modes in the spectra of $\sigma(H_{k,i,\phi})$, on the one hand, and $\sigma(H_{k,2,\phi})$, on the other hand. Whereas $\times$ denotes the absence of zero modes, the entries $\circ$ or $\otimes$ in the last two columns denote the presence of zero modes with or without spectral flow, respectively, in the spectra of $\sigma(Q_{k,1,\phi} A_{i+1})$, on the one hand, and $\sigma(Q_{k,2,\phi} A_{i+1})$, on the other hand.

column of Table 6.4 as one varies ($\mathcal{R}, \mathcal{H}$). For a given row in Table 6.4 $V_{\phi,\phi}$ is contained in the most general perturbation $V_{\phi}$ that is compliant with the AIII symmetry. We define the single-particle Hamiltonian $H_{i,\phi,\phi} = H_i + V_{\phi,\phi}$ by its matrix elements

$$H_{k,i,\phi} r_{i+1} r'_{i+1} := H_{k,i+1} r_{i+1} r'_{i+1} + V_{\phi,\phi} r_{i+1} r'_{i+1},$$

(6.162a)

$$V_{\phi,\phi} r_{i+1} r'_{i+1} := \delta_{r_{i+1}, r'_{i+1}} \sum_{\mu, \nu \in \text{row}} v_{\mu \nu} X_{\mu \nu}.$$

(6.162b)

The corresponding equal-time one-point correlation matrix is $Q_{\phi,\phi} (i+1)$ and its upper-left block is $Q_{\phi,\phi} A_{i+1}$. The third column in Table 6.4 provides one sign for each row. The sign $\eta_\phi$ is positive if $\phi$ commutes with $\phi$ and negative if $\phi$ anti-commutes with $\phi$. The information contained in $\eta_\phi$ is needed to read from Table VI of Ref. [161] the bulk topological index of the single-particle Hamiltonian (6.162). This topological index does not guarantee that $H_{\mathcal{R},\phi}$ supports boundary states in an open geometry. On the other hand, $Q_{\mathcal{R},\phi} A_{i+1}$ supports boundary states on the entangling boundaries. The entries $\circ$ for the columns $\sigma(H_{k,i,\phi})$ and $\sigma(Q_{k,i,\phi} A_{i+1})$ are a consequence of our stability analysis. On the one hand, Table 6.4 demonstrates explicitly that the presence of a reflection symmetry in addition to the chiral symmetry does not guarantee that a non-vanishing bulk topological index implies protected edge states in the spectrum $\sigma(H_{k,i,\phi})$ for both edges $i = 1, 2$. On the other hand, Table 6.4 demonstrates explicitly that a non-vanishing bulk topological index always implies protected entangling states in the spectrum $\sigma(Q_{k,i,\phi} A_{i+1})$ irrespective of the choice $i = 1, 2$ made for the entangling boundary.
6.5.5 Existence of spectral flows in the entanglement spectra

We are going to study the dependences of the spectra $\sigma(\mathcal{H}_{k_1,\mathcal{R}_2;\mathcal{S}})$ and $\sigma(Q_{k_1,\mathcal{R}_2;\mathcal{S}} A_{i+1})$ (with $i + 1$ defined modulo 2) on the system sizes for the single-particle Hamiltonian $\mathcal{H}_{k_1,\mathcal{R}_2;\mathcal{S}}$ defined by the matrix elements (6.162) and the corresponding upper-left block $Q_{k_1,\mathcal{R}_2;\mathcal{S}} A_{i+1}$ from the equal-time one-point correlation matrix. Without loss of generality, we will present numerical results obtained by choosing the fifth row in Table 6.4 to define $\mathcal{H}_{k_1,\mathcal{R}_2;\mathcal{S}}$ and $Q_{k_1,\mathcal{R}_2;\mathcal{S}} A_{i+1}$ with $(v_{02}, v_{03}, v_{12}, v_{13}) = (0.2, -0.1, 0.05, 0.3)$.

The question we want to address is the following. On the one hand, Figs. 6.5(a-d) suggest that the mid-gap branches merge into the continuum when $\pi/2 < |k_i| < \pi$. On the other hand, the mid-gap branches in Fig. 6.5(e)
seem to be separated by a very small gap from all other bands in the vicinity of $|k_1| = \pi$, while no gap is resolved in energy between the mid-gap branches and all other branches in the vicinity of $|k_1| = \pi$ for Figs. 6.5(f-h).

The first question we are going to address is how to interpret the “peeling of” the mid-gap branches from the continua in Figs. 6.5(a-d). To this end, we present in Fig 6.7(a) the spectrum $\sigma(H_{k_1;\vec{r}_1;\vec{r}})$ obtained by imposing periodic boundary conditions along the direction $i = 1$ and open boundary conditions along the direction $i + 1 = 2$ for the linear system sizes $M_1 = 128$ and $M_2 = 64$. We then compute the spectrum of $H_{k_1;\vec{r}_1;\vec{r}}$ for each value $M_2 = 16, 32, 48, 64, 80, 96$ of the cylinder height. At last, we compute the minimal value $\Delta_{\min}(\pi/2, M_2) > 0$ taken by the difference in energy between the positive energy eigenvalues at $k_1 = \pi/2$ from any one of the bulk bands and the mid-gap branch with positive energy eigenvalue at $k_1 = \pi/2$. The dependence of this direct gap $\Delta_{\min}(\pi/2, M_2) > 0$ on $M_2 = 16, 32, 48, 64, 80, 96$ holding $M_1 = 128$ fixed is plotted in Fig 6.7(b). The fast decrease of $\Delta_{\min}(\pi/2, M_2) > 0$ with increasing values of $M_2 = 16, 32, 48, 64, 80, 96$ holding $M_1 = 128$ fixed is interpreted as the merging of the mid-gap branch into the continuum of conduction bulk states in the quasi-one-dimensional limit $M_2 \to \infty$ holding $M_1 = 128$ and $\pi/2 \leq k_1 \leq \pi$ fixed. Similarly, one may verify that the mid-gap branches merge into the valence and conduction bulk continua in Figs. 6.5(a-d) for a non-vanishing interval of momenta $k_i$ in the quasi-one-dimensional limit $M_{i+1} \to \infty$ holding $M_i$ fixed. If we change the conserved momentum $k_i$ adiabatically, say by imposing twisted boundary conditions instead of periodic ones along the $i$ direction, a charge can be transferred from the valence bulk continuum to the conduction bulk continuum through the mid-gap branches. This is an example of spectral flow induced by mid-gap states crossing a bulk gap.

The same quasi-one-dimensional scaling analysis, when performed on the spectra $\sigma(H_{k_2;\vec{r}_2;\vec{r}})$ and $\sigma(Q_{k_1;\vec{r}_1;\vec{r}}A_2)$, delivers a very different result. First, the mid-gap branches of $H_{k_2;\vec{r}_2;\vec{r}}$ fail to cross. Second, the minimal value $\Delta_{\min}(\pi, M_2) > 0$ taken by the difference between the positive eigenvalues at $k_1 = \pi$ from any one of the bulk bands and the mid-gap branch with positive energy eigenvalues at $k_1 = \pi$ converge to a non-vanishing value upon increasing $M_2 = 16, 32, 48, 64, 80, 96$ holding $M_1 = 128$ fixed in Fig 6.7(c). Instead of plotting the evidence for the saturation value $\lim_{M_2 \to \infty} \Delta_{\min}(\pi, M_2) > 0$, we plot in Fig 6.7(d) the entanglement spectrum

$$\varpi_{k_1} := \ln \left( \frac{1}{\zeta_{k_1}} - 1 \right),$$

which we already encountered in Eq. (6.14).

We now reproduce Figs 6.7(c) and Fig 6.7(d) for $M_1 = 64$ and $M_2 = 128$ with the single change that we choose the geometry in which it is $k_2$ instead of $k_1$ that is chosen to be the good quantum number. There follows Figs 6.7(e) and Fig 6.7(f) for $\sigma(Q_{k_2;\vec{r}_2;\vec{r}}A_1)$ and $\sigma \left( \ln(Q_{k_2;\vec{r}_2;\vec{r}}A_1^{-1}) \right)$, respectively. We have verified that, if we increase simultaneously $M_1$ and $M_2$, there is a level crossing between the mid-gap branches and the bulk branches in the
neighborhood of ±π. The existence of this level crossing is implied by the coloring of the bands in Fig 6.7(f). This coloring has the following origin.

For any row from Table 6.4 we may construct the operator

\[ \Lambda_{k_2 \mathcal{A}_{A_1+1}} := \Gamma_{k_2 \mathcal{R}} S_{A_{A_1+1}} \] (6.164)

whenever the reflection \( \mathcal{R} \) is block off-diagonal with respect to the partition. Here, \( \Gamma_{k_2 \mathcal{R}} \) was defined in Eq. (6.46), while the representation \( S \) of the chiral operation \( \mathcal{S} \) is diagonal in the partition with the upper-left block \( S_{A_{A_1+1}} \).

For the fifth row from Table 6.4, \( \Gamma_{k_1 \mathcal{R}_2} \) does not exist in the geometry that defines \( Q_{k_1 \mathcal{R}_2: \mathcal{A}_{A_2}} \), since \( \mathcal{R}_2 \) is block diagonal for this partition. For the fifth row from Table 6.4, \( \Gamma_{k_2 \mathcal{R}_2} \) exists in the geometry that defines \( Q_{k_2 \mathcal{R}_2: \mathcal{A}_{A_1}} \) and anti-commutes with \( Q_{k_2 \mathcal{R}_2: \mathcal{A}_{A_1}} \) according to Eq. (6.53), since \( \mathcal{R}_2 \) is block off-diagonal for this partition. Hence, \( \Lambda_{k_2 \mathcal{A}_{A_1}} \) commutes with \( Q_{k_2 \mathcal{R}_2: \mathcal{A}_{A_1}} \) and we may associate to any eigenstate of \( Q_{k_2 \mathcal{R}_2: \mathcal{A}_{A_1}} \) an eigenvalue of \( \Lambda_{k_2 \mathcal{A}_{A_1}} \). This eigenvalue of \( \Lambda_{k_2 \mathcal{A}_{A_1}} \) is complex valued as \( \Lambda_{k_2 \mathcal{A}_{A_1}} \) is not necessarily Hermitian. It turns out that \( \Lambda_{k_2 \mathcal{A}_{A_1}} \) is purely imaginary according to our exact diagonalizations. The coloring in Fig 6.7(f) corresponds to the sign of the imaginary eigenvalue of \( \Lambda_{k_2 \mathcal{A}_{A_1}} \). This quantum number rules out an avoided level crossing of the mid-gap branches in the neighborhood of \( k_2 = 0 \) in Fig 6.7(f). This quantum number also rules out an avoided level crossing at the zone boundary \( k_2 = \pi \). Inspection of the colored dispersions in Fig 6.7(f) suggests that twisting boundary conditions induces a spectral flow from the valence to the conduction bands through the mid-gap branches. This is the basis of the distinction between crossings of mid-gap branches that are compatible with a spectral flow and are denoted by \( \circ \) in Table 6.4 and crossing of mid-gap branches that are not compatible with a spectral flow and are denoted by \( \otimes \) in Table 6.4.

In summary, we can understand the fifth row from Table 6.4 (an all remaining rows with the same reasoning) as follows. Because the reflection and chiral operations commute, the topological index of a generic Hamiltonian obeying these two symmetries belongs to \( \mathbb{Z} \). Protected edge states can but need not be present in the spectrum of the Hamiltonian in a cylindrical geometry. Protected edge states arise if and only if the disconnected boundaries are not mixed by the reflection symmetry, i.e., for \( \mathcal{H}_{k_1 \mathcal{R}_2: \mathcal{A}_2} \) but not for \( \mathcal{H}_{k_2 \mathcal{R}_2: \mathcal{A}_2} \). On the other hand, the upper-left block \( Q_{k_1 \mathcal{R}_2: \mathcal{A}_2} \) and \( Q_{k_2 \mathcal{R}_2: \mathcal{A}_1} \) of the equal-time correlation matrix both have robust mid-gap branches that cross. However, it is only the mid-gap branches of \( Q_{k_2 \mathcal{R}_2: \mathcal{A}_1} \) that support a spectral flow between the valence and conduction continua, for it is only then that the reflection \( \mathcal{R}_2 \) is block off-diagonal in the partition defined by \( A_1 \). The fifth row from Table 6.4 demonstrates that topological protection can be absent from the spectrum of the Hamiltonian but present in the spectrum of the equal-time correlation matrix.
6.6 Topological band insulator protected by two reflection symmetries in two dimensions

6.6.1 Hamiltonian and topological quantum numbers

Our third example is defined by choosing $d = 2$ and $N_{\text{orb}} = 2$ in Eq. (6.2). We consider the two-dimensional plane $z = 0$ from the three-dimensional Cartesian space $\mathbb{R}^3 := \{ x, y, z | x, y, z \in \mathbb{R} \}$ with the orthonormal basis $x, y,$ and $z$. The single-particle Hamiltonian is defined by (the convention $e > 0$ is used for the electron charge)

$$\hat{H} := \sum_{\sigma = \pm} \frac{\hbar^2}{2m} \left[ \hat{p}_\sigma - \frac{e}{c} A(\hat{r}) \sigma_3 \right]^2$$  \hspace{1cm} (6.165a)

where $\sigma_0$ for the $2 \times 2$ unit matrix and $\sigma$ for the Pauli matrices are the usual suspects,

$$\hat{p} := \begin{pmatrix} \hat{p}_x \\ \hat{p}_y \end{pmatrix}$$  \hspace{1cm} (6.165b)

is the momentum operator in the plane $z = 0$,

$$\hat{r} := \begin{pmatrix} \hat{r}_x \\ \hat{r}_y \end{pmatrix}$$  \hspace{1cm} (6.165c)

is the position operator in the plane $z = 0$, and $A(\hat{r})$ is the classical electromagnetic vector potential such that

$$(\nabla \wedge A)(r) = Bz$$  \hspace{1cm} (6.165d)

is the uniform magnetic of magnitude $B > 0$ pointing along $z$. This model describes an electron; with mass $m$, electric charge $-e$, and the conserved spin quantum number along the quantization axis defined by the eigenstates of the Pauli matrix $\sigma_3$; undergoing the spin quantum Hall effect generated by the matrix-valued field $B\sigma_3 z$.

The eigenvalue spectrum consists of Landau levels with the single-particle energy eigenvalues

$$\varepsilon_n = \hbar \omega_c \left( n + \frac{1}{2} \right), \quad n = 0, 1, 2, \cdots$$  \hspace{1cm} (6.166a)

where

$$\omega_c := \frac{eB}{mc}$$  \hspace{1cm} (6.166b)

is the cyclotron frequency. In addition to the usual orbital degeneracy $\Phi/\Phi_0$ of Landau levels with $\Phi$ the total mag-
netic flux and $\Phi_0 := h c / e$ the flux quantum, there is the Kramers’ degeneracy under the composition of complex conjugation and conjugation by $\sigma_2$.

Each Landau level fully filled by $\Phi / \Phi_0$ electrons with spin up carries the Chern number $C_+ = +1$. Each Landau level fully filled by $\Phi / \Phi_0$ electrons with spin down carries the Chern number $C_- = -1$. The contribution to the Hall conductivity from any completely filled Landau level is therefore

$$\sigma_{QHE} = \left( C_+ + C_- \right) \frac{e^2}{h} = 0. \quad (6.167a)$$

The contribution to the spin Hall conductivity from any completely filled Landau level is

$$\sigma_{SQHE} = \frac{\hbar}{2e} \left( C_+ - C_- \right) \frac{e^2}{h} = \frac{e}{2\pi}. \quad (6.167b)$$

On an infinite strip along the $x$ direction of width $L_y$ along the $y$ direction, we impose translation symmetry along the $y$ direction through periodic boundary conditions. For this cylindrical geometry (recall Fig. 6.6 with the identification $i = y$ and $i + 1 = x$), it is convenient to choose the Landau gauge

$$A := B \begin{pmatrix} 0 \\ x \end{pmatrix} \quad (6.168a)$$

for which normalized single-particle eigenstates $|n, \sigma, k_y\rangle$ in the lowest Landau level $n = 0$ can be represented by the normalized eigen-wavefunctions in the lowest ($n = 0$) Landau levels

$$\langle x, y | n = 0, \sigma, k_y \rangle \equiv f_{k_y}^{(\sigma)}(x, y) = \frac{e^{+ik_y y} e^{-(x-\sigma \ell_B^2 k_y)/(2\ell_B^2)}}{(\sqrt{\pi} \ell_B L_y)^{1/2}} \quad (6.168b)$$

for a spin $\sigma$ electron. Here, $\sigma = \pm$ is the spin of the electron along the quantization axis, $r = (x, y) \in \mathbb{R}^2$ is the coordinate of the electron, and

$$k_y = \frac{2\pi}{L_y} m, \quad m = 1, \ldots, \frac{\Phi}{\Phi_0}, \quad (6.168c)$$

is the quantized wave number arising from the compactification along the width $L_y$ of the strip and

$$\ell_B := \sqrt{\frac{\hbar c}{eB}} \quad (6.168d)$$

is the magnetic length that we shall set to unity from now on.
6.6.2 Symmetries

The symmetries of the single-particle Hamiltonian defined by Eq. (6.165) are the following.

1. Let $R_x$ define the reflection about the horizontal axis $r = (x, 0)$ by which the quantum numbers of the position and momentum operators transform according to

\[
R_x : x \mapsto +x, \quad R_x : y \mapsto -y,
\]

\[
R_x : k_x \mapsto +k_x, \quad R_x : k_y \mapsto -k_y,
\]

respectively. The symmetry

\[
\hat{O}_x^\dagger \hat{H} \hat{O}_x = \hat{H}
\]

then holds for the single-particle Hamiltonian (6.165) if $R_x$ is represented by the composition of $x \mapsto +x$, $y \mapsto -y$ with the conjugation by either $\sigma_x$ or $\sigma_y$. We choose the representation

\[
\hat{O}_x \chi_{k_y}(x, y) := \sigma_x \chi_{-k_y}(x, -y)
\]

for any two-component spinor $\chi_{k_y}(x, y) \in \mathbb{C}^2$.

2. Let $R_y$ define the reflection about the vertical axis $r = (0, y)$ by which the quantum numbers of the position and momentum operators transform according to

\[
R_x : x \mapsto -x, \quad R_x : y \mapsto +y,
\]

\[
R_x : k_x \mapsto -k_x, \quad R_x : k_y \mapsto +k_y,
\]

respectively. The symmetry

\[
\hat{O}_y^\dagger \hat{H} \hat{O}_y = \hat{H}
\]

then holds for the single-particle Hamiltonian (6.165) if $R_y$ is represented by the composition of $x \mapsto -x$, $y \mapsto +y$ with the conjugation by $\sigma_x$, given the choice made in Eq. (6.169c), i.e.,

\[
\hat{O}_y \chi_{k_y}(x, y) := \sigma_x \chi_{k_y}(-x, y)
\]

for any two-component spinor $\chi_{k_y}(x, y) \in \mathbb{C}^2$. With this choice, the commutation relation $[\hat{R}_x, \hat{R}_y] = 0$ is faithfully represented, i.e.,

\[
[\hat{O}_x, \hat{O}_y] = 0.
\]
3. Let \( \mathcal{T} \) define reversal of time by which time and the quantum numbers of the position and momentum operators transform according to

\[
\mathcal{T} : t \mapsto -t, \\
\mathcal{R}_x : x \mapsto x, \quad \mathcal{R}_x : y \mapsto y, \\
\mathcal{R}_x : k_x \mapsto -k_x, \quad \mathcal{R}_x : k_y \mapsto -k_y,
\]

respectively. The symmetry

\[
\hat{O}_\mathcal{T} \hat{H} \hat{O}_\mathcal{T} = \hat{H}
\]

then holds for the single-particle Hamiltonian (6.165a) if \( \mathcal{T} \) is represented by the composition of charge conjugation with the conjugation by \( \sigma_x \), i.e.,

\[
\hat{O}_\mathcal{T} \chi_{k_y}(x,y) := \sigma_x \chi_{-k_y}(x,y)
\]

for any two-component spinor \( \chi_{k_y}(x,y) \in \mathbb{C}^2 \). With this choice, the commutation relations \([\mathcal{R}_x, \mathcal{T}] = 0\) are faithfully represented, i.e.,

\[
[\hat{O}_\mathcal{T}, \hat{O}_{\mathcal{R}_x}] = [\hat{O}_\mathcal{T}, \hat{O}_{\mathcal{R}_y}] = 0.
\]

Observe that had we implemented the two reflections by choosing \( \sigma_y \) instead of \( \sigma_x \) on the right-hand sides of Eqs. (6.169c) and (6.170c), then the transformation of reversal of time would anti-commute with both reflections.
6.6.3 Partition and zero modes

The counterpart to the projection of $\hat{\psi}_i^\dagger \hat{\psi}_j$ in the equal-time one-point correlation matrix (6.6) onto the completely filled Landau level $n = 0$ is the operator

$$\hat{C} = \sum_{\sigma = \pm} \sum_{L_y k_y/(2\pi) = 1} \hat{C}_\sigma \equiv \sum_{\sigma = \pm} \sum_{L_y k_y/(2\pi) = 1} |n = 0, \sigma, k_y\rangle \langle n = 0, \sigma, k_y|$$

(6.174a)

with the matrix element

$$C_{\sigma, k_y} (x, x') \equiv \langle n = 0, \sigma, k_y, x|\hat{C}|n = 0, \sigma, k_y, x'\rangle = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2}[(x - \sigma k_y)^2 + (x' - \sigma k_y)^2]}$$

(6.174b)

for any $x, x' \in \mathbb{R}$. One verifies that the $2 \times 2$ matrix

$$\hat{C}_k (x, x') := C_{+, k_y} (x, x') \sigma_{11} + C_{-, k_y} (x, x') \sigma_{22},$$

(6.175a)

where $\sigma_{11} := (\sigma_0 + \sigma_3)/2$ and $\sigma_{22} := (\sigma_0 - \sigma_3)/2$, obeys

$$\hat{O}_{\sigma}^\dagger \hat{C}_{-k_y} (x, x') \hat{O}_{\sigma} = \hat{C}_{k_y} (x, x'),$$

(6.175b)

$$\hat{O}_{\sigma_y}^\dagger \hat{C}_{k_y} (-x, -x') \hat{O}_{\sigma_y} = \hat{C}_{k_y} (x, x'),$$

(6.175c)

$$\hat{O}_{\sigma_y'}^\dagger \hat{C}_{-k_y} (x, x') \hat{O}_{\sigma_y'} = \hat{C}_{k_y} (x, x').$$

(6.175d)

We define the partition

$$A := \left\{ \sigma, k_y, x \mid \sigma = \pm, k_y = \frac{2\pi}{L_y}, \ldots, \frac{2\pi \Phi}{L_y \Phi_0}, x < 0 \right\}$$

(6.176a)

and

$$B := \left\{ \sigma, k_y, x \mid \sigma = \pm, k_y = \frac{2\pi}{L_y}, \ldots, \frac{2\pi \Phi}{L_y \Phi_0}, x > 0 \right\}$$

(6.176b)

for the single-particle labels. The restriction of the equal-time one-point correlation operator defined by Eq. (6.174) to $x < 0$ and $x' < 0$ defines the operator $\hat{C}_A$ with its matrix elements $C_{\sigma, k_y A} (x, x')$ and the $2 \times 2$ matrix $\hat{C}_{k_y A} (x, x')$. The restriction of the equal-time one-point correlation operator defined by Eq. (6.174) to $x > 0$ and $x' > 0$ defines the operator $\hat{C}_B$ with its matrix elements $C_{\sigma, k_y B} (x, x')$ and the $2 \times 2$ matrix $\hat{C}_{k_y B} (x, x')$. With this partition, for any...
\[ x, x' < 0, \]

\[
\hat{O}_{x}^1 \hat{C}_{-k_y A}(x, x') \hat{O}_{x} = \hat{C}_{-k_y A}(x, x'), \tag{6.177a}
\]

\[
\hat{O}_{y}^1 \hat{C}_{k_y A}(x, x') \hat{O}_{y} = \hat{C}_{k_y B}(-x, -x'), \tag{6.177b}
\]

\[
\hat{O}_{y}^1 \hat{C}_{-k_y A}(x, x') \hat{O}_{y} = \hat{C}_{k_y A}(x, x'). \tag{6.177c}
\]

The same equations hold if we do \( x \rightarrow -x, x' \rightarrow -x', A \rightarrow B, \) and \( B \rightarrow A \). The restriction of the equal-time one-point correlation operator defined by Eq. (6.174) to \( x < 0 \) and \( x' > 0 \) defines the operator \( \hat{C}_{AB} \) with its matrix elements \( C_{\sigma,k_y}^{AB}(x,x') \), and the \( 2 \times 2 \) matrix \( \hat{C}_{k_y}^{AB}(x,x') \). Finally, the restriction of the equal-time one-point correlation operator defined by Eq. (6.174) to \( x > 0 \) and \( x' < 0 \) defines the operator \( \hat{C}_{BA} = \hat{C}_{AB}^\dagger \) with its matrix elements \( C_{\sigma,k_y}^{BA}(x,x') \) and the \( 2 \times 2 \) matrix \( \hat{C}_{k_y}^{BA}(x,x') = \hat{C}_{k_y}^{AB}(x',x) \).

The normalizable eigenstates of \( \hat{C}_{k_y}^{A} \) are represented by

\[
\phi_{+,k_y}(x) = \frac{1}{\sqrt{2 \pi^{1/4}}} \begin{pmatrix} e^{-\frac{1}{2}(x-k_y)^2} \\ 0 \end{pmatrix} \tag{6.178}
\]

and

\[
\phi_{-,k_y}(x) = \frac{1}{\sqrt{2 \pi^{1/4}}} \begin{pmatrix} 0 \\ e^{-\frac{1}{2}(x+k_y)^2} \end{pmatrix} \tag{6.179}
\]

for any \(-\infty < x \leq 0\. In the thermodynamic limit \( L_y \rightarrow \infty \) holding the electron density fixed, the corresponding eigenvalues are given by

\[
\zeta_{\pm}(k_y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{0} dx \ e^{-(x \mp k_y)^2} = \frac{1}{2} \left[ 1 - \text{erf}(\pm k_y) \right]. \tag{6.180}
\]

The spectrum \( 1 - 2 \zeta_{\pm}(k_y) \) of

\[
\hat{Q}_{k_y} := \hat{1} - 2 \hat{C}_{k_y A} \tag{6.181}
\]

is shown in Fig. 6.8. Two chiral edge modes of opposite chirality are seen crossing the spectrum with a crossing at vanishing entanglement eigenvalue.

On the one hand, Eqs. (6.177a) and (6.177c) imply that the reflection about the horizontal axis (6.169) and reversal of time (6.172) are represented by the operators \( \hat{O}_{x}^\dagger \) and \( \hat{O}_{y}^\dagger \), respectively, that are block diagonal with respect to the partition of the single-particle labels into the sets \( A \) and \( B \) defined by Eq. (6.176). As explained in Eqs. (6.38) and (6.39), the upper-left block (6.181) inherits these symmetries from \( \hat{H} \) defined in Eq. (6.165).
On the one hand, Eq. (6.177b) implies that \( \hat{O} \) is block off diagonal with respect to the partition of the single-particle labels into the sets \( A \) and \( B \) defined by Eq. (6.176). The counterparts to Eqs. (6.40) and (6.41) then hold, so that we may apply the counterpart to the spectral symmetry (6.46).

To proceed, for any \( x, x' < 0 \) and \( k_y, k'_y = 2\pi/L_y, \cdots, (2\pi \Phi)/(L_y \Phi_0) \), we make use of the representations

\[
\hat{O}_{k_y,k'_y} \mathcal{R}_x A(x, x') := \langle k_y, x| \hat{O} |k'_y, x'\rangle = \delta_{k_y,k'_y} \delta(x - x') \sigma_x, \tag{6.182}
\]

for the reflection about the horizontal axis,

\[
\hat{O}_{k_y,k'_y} \mathcal{R}_y A(x, x') := \langle k_y, x| \hat{O} |k'_y, x'\rangle = \delta_{k_y,k'_y} \delta(x + x') \sigma_x, \tag{6.183}
\]

for the reflection about the vertical axis, and

\[
\hat{O}_{k_y,k'_y} \mathcal{T}_A(x, x') := \langle k_y, x| \hat{O} |k'_y, x'\rangle = \delta_{k_y,k'_y} \delta(x - x') \sigma_y K, \tag{6.184}
\]

for the reversal of time (\( K \) denotes complex conjugation). Consequently, the upper-left block (6.181) obeys the symmetries

\[
\hat{Q}_{k_y} A(x, x') = \sum_{k''_y} \sum_{k'''_y} \int_{-\infty}^{0} dx'' \int_{-\infty}^{0} dx'''
\]

\[
\hat{O}^\dagger_{k_y,k''_y} \mathcal{R}_x A(x, x'') \delta_{k''_y,k'''_y} \hat{Q}_{k''_y} A(x'', x''') \hat{O}_{k'''_y,k'_y} \mathcal{R}_x A(x''', x')
\]

\[
= \sigma_x \hat{Q}_{-k_y} A(x, x') \sigma_x \tag{6.185a}
\]

under reflection about the horizontal axis and

\[
\hat{Q}_{k_y} A(x, x') = \sum_{k''_y} \sum_{k'''_y} \int_{-\infty}^{0} dx'' \int_{-\infty}^{0} dx'''
\]

\[
\hat{O}^\dagger_{k_y,k''_y} \mathcal{T}_A(x, x'') \delta_{k''_y,k'''_y} \hat{Q}_{k''_y} A(x'', x''') \hat{O}_{k'''_y,k'_y} \mathcal{T}_A(x''', x')
\]

\[
= \sigma_y \hat{Q}_{-k_y} A(x, x') \sigma_y \tag{6.185b}
\]

under reversal of time. The symmetry of the Hamiltonian (6.165a) under reflection about the vertical axis is turned
into the spectral symmetry

$$
\hat{Q}_{k_y} A(x, x') = \sum_{k''_y} \int_{-\infty}^{0} dx'' \int_{-\infty}^{0} dx'''
\hat{\Gamma}^\dagger_{k_y, k''_y} \delta_{k''_y, k'_y} \hat{Q}_{k'_y} A(x'', x''') \hat{\Gamma}^\dagger_{k'_y, k''_y} A(x''', x') \tag{6.186a}
$$

where

$$
\hat{\Gamma}_{k_y, k'_y} A(x, x') = \sum_{k''_y}^\infty \int_{0}^{+\infty} dx'' \delta_{k_y, k''_y} \hat{C}_{k_y} A(x, x'') \hat{O}^\dagger_{k''_y, k'_y} A(x'', x')
\tag{6.186b}
$$

$$
= \delta_{k_y, k'_y} \frac{1}{\sqrt{\pi}} \left[ e^{-\frac{1}{2}[(x-k_y)^2+(x'+k_y)^2] \sigma_{12}} + e^{-\frac{1}{2}[(x+k_y)^2+(x'-k_y)^2] \sigma_{21}} \right]
$$

with $\sigma_{12} := (\sigma_1 + i \sigma_2)/2$ and $\sigma_{21} := (\sigma_1 - i \sigma_2)/2$. For any $x < 0$ and $k_y = 2\pi/L_y$, ···, $(2\pi \Phi)/(L_y \Phi_0)$, one verifies the eigenvalue equation

$$
\sum_{k''_y} \int_{-\infty}^{0} dx' \hat{\Gamma}_{k_y, k'_y} A(x, x') \phi_{\pm, k''_y}(x') = \frac{1}{2} \left[ 1 - \text{erf}(k_y) \right] \phi_{\mp, k_y}(x). \tag{6.187}
$$

### 6.6.4 Stability analysis of the zero modes

We are after the stability of the crossings at vanishing energy and momentum that characterizes the edge states in the Hamiltonian defined by Eq. (6.165) for a cylindrical geometry and the states in the entanglement spectra localized on the entangling boundary at $x = 0$ defined in Sec. 6.6.3. We are going to show that the reflection symmetries $R_x$ and $R_y$ do not protect the edge states on the physical boundaries, but they protect the edge states on the entangling boundary.

#### Hamiltonian spectrum

If we linearize the edge state spectrum close to vanishing energy and momentum, we get the effective Hamiltonian (the group velocity has been set to one)

$$
\hat{H}_{\text{edges}}(k_y) \approx k_y Y_{33} \tag{6.188}
$$

in the cylindrical geometry of Fig. 6.6 ($i = y$ and $i + 1 = x$), where we have introduced a second set of $2 \times 2$ matrices generated by the unit $2 \times 2$ matrix $\rho_0$ on the Pauli matrices $\rho_1$, $\rho_2$, and $\rho_3$ when defining

$$
Y_{\mu\nu} := \sigma_\mu \otimes \rho_\nu \tag{6.189}
$$
for $\mu, \nu = 0, 1, 2, 3$. The matrices $\rho_0$, $\rho_1$, $\rho_2$, and $\rho_3$ encode the mixing of edge states localized on opposite edges of the cylinder. Reflection about the $x$ axis, reflection about the $y$ axis, and reversal of time are represented by

\[
\hat{O}_{\text{edges} \, R_x}(k_y, k'_y) := \delta(k_y - k'_y) Y_{11}, \quad (6.190b)
\]

\[
\hat{O}_{\text{edges} \, \mathcal{T}}(k_y, k'_y) := \delta(k_y + k'_y) Y_{20} K, \quad (6.190c)
\]

where $K$ denotes charge conjugation. In a gradient expansion, any perturbation of the form

\[
\hat{V}_{\text{edges} \, \mu\nu} = v_{\mu\nu} Y_{\mu\nu} \quad (6.191)
\]

for some energy scale $v_{\mu\nu} \in \mathbb{R}$ that is smaller than the cyclotron energy, commutes with the three transformations (6.190), and anti-commutes with $Y_{33}$, say $\hat{V}_{\text{edges} \, 01}$, opens a spectral gap on the edges.

In the thermodynamic limit by which the length of the cylinder is taken to infinity keeping the density of electrons fixed, there is no mixing between edge states localized on opposite boundaries of the cylinder. The effective Hamiltonian on a single edge becomes

\[
\hat{H}_{\text{edge}}(k_y) \approx k_y \sigma_3. \quad (6.192)
\]

It commutes with

\[
\hat{O}_{\text{edge} \, R_x}(k_y, k'_y) := \delta(k_y + k'_y) \sigma_1, \quad (6.193a)
\]

\[
\hat{O}_{\text{edge} \, \mathcal{T}}(k_y, k'_y) := \delta(k_y + k'_y) \sigma_2 K, \quad (6.193b)
\]

where $K$ denotes charge conjugation. In a gradient expansion, a generic perturbation on this single edge is of the form

\[
\hat{V}_{\text{edge}} = \sum_{\mu=0}^{3} v_{\mu} \sigma_{\mu} \quad (6.194)
\]

with any $v_{\mu} \in \mathbb{R}$ much smaller than the bulk gap.

Imposing reflection symmetry enforces the conditions $v_2 = v_3 = 0$ on the perturbation $\hat{V}_{\text{edge}}$, i.e., a reflection symmetric perturbation can open a gap at the crossing in the unperturbed spectrum. The crossing in the unperturbed spectrum of a single edge is thus not protected by having two reflection symmetries in the bulk Hamiltonian. This is not true anymore for the entanglement spectrum.

Imposing time-reversal symmetry enforces the conditions $v_1 = v_2 = v_3 = 0$ on the perturbation $\hat{V}_{\text{edge}}$, i.e., a
time-reversal symmetric perturbation does not destroy the crossing, it merely shifts the crossing in the unperturbed spectrum at vanishing momentum to a non-vanishing energy.

**Entanglement spectrum**

In the thermodynamic limit by which the length of the cylinder is taken to infinity keeping the density of electrons fixed, there is no mixing between states localized on the physical boundaries at \( x = \pm \infty \) and the entangling boundary at \( x = 0 \). The entangling edge states close to the crossing at vanishing entangling eigenvalue and momentum of Fig. 6.8 are governed by the effective Hamiltonian (the group velocity has been set to one)

\[
\hat{Q}_{\text{edge}}(k_y) \approx k_y \sigma_3. 
\]  
(6.195)

The representations of the two symmetry transformations (6.193a) and (6.193b) remain valid. In addition, the spectral symmetry transformation (6.186) takes the form of an anti-commutation with

\[
\hat{\Gamma}_{\text{edge,R}}(k_y, k'_y) \propto \delta(k_y - k'_y) \sigma_1
\]  
(6.196)
when \( x = x' = 0 \) and \( k_y, k'_y \approx 0 \). A perturbation of the form (6.194) is then restricted to the conditions \( v_2 = v_3 = 0 \) if it commutes with the generator (6.193a) for reflection about the horizontal axis. A perturbation of the form (6.194) is restricted to the conditions \( v_0 = v_1 = 0 \) if it anti-commutes with the generator (6.196) for reflection about the vertical axis. Imposing both reflection symmetries on the Hamiltonian thus protects the crossing at vanishing entangling eigenvalue and momentum in Fig. 6.8 from any perturbation, unlike for the crossing at vanishing energy and momentum of the edge states for the Hamiltonian.

Finally, a perturbation of the form (6.194) is restricted to the conditions \( v_1 = v_2 = v_3 = 0 \) if it commutes with the generator (6.193b) for reversal of time. Imposing time-reversal symmetry on the Hamiltonian thus protects the existence of a crossing at vanishing momentum in Fig. 6.8 from any perturbation.

### 6.7 Graphene with Kekule order as an inversion-symmetric topological insulator in two dimensions

#### 6.7.1 Introduction

Graphene has two single-particle bands that touch linearly at two inequivalent points \( K \) and \( K' \) from the first Brillouin zone of the triangular lattice (BZT). These two inequivalent points from the BZT of graphene are called
Dirac points. If graphene is modeled by a tight-binding model with two bands, whereby spinless electrons can only hop with a uniform amplitude $t$ between the nearest-neighbor sites of the honeycomb lattice, then the linear band touching is located at the two inequivalent corners of the hexagonal BZT of graphene. Graphene is a planar semi-metal with a low-energy and long-wave length electronic structure that can be modeled by a $4 \times 4$ massless Dirac Hamiltonian in $(2 + 1)$-dimensional space and time. The rank four of the Dirac matrices entering this Dirac Hamiltonian arises because only the two bands with a linear touching are kept in the low-energy sector of graphene and after linearization of the single-particle spectrum about the two Dirac points $K$ and $K'$.

The Kekule distortion is a pattern of symmetry breaking on the honeycomb lattice by which the nearest-neighbor hopping amplitude takes the two distinct real values $t_1$ and $t_2$, respectively. This pattern of symmetry breaking is depicted in Fig. 6.9(a) through the coloring of the nearest-neighbor bonds of the honeycomb lattice. The Kekule distortion is weak if $|t_1 - t_2| \ll |t_1 + t_2|/2$, in which case a single-particle gap $\Delta_K \propto |t_1 - t_2|$ that is much smaller than the band width ($\propto |t_1 + t_2|/2$) opens up a the Dirac points. A Kekule distortion can be induced by fine-tuning of sufficiently large repulsive interactions. A Kekule distortion is also favored in the presence of a sufficiently large magnetic field by some phonons. A Kekule distortion may also arise locally at the core of a vortex in the (proximity-induced) superconducting phase of graphene. Finally, a Kekule distortion has been observed in artificial graphene (molecular graphene) obtained by patterning carbon monoxide molecules on the 111 surface of copper.

A distinctive feature of graphene is a density of states that vanishes linearly if single-particle energies are measured relative to the energy of the Dirac points at sufficiently small energies. This semi-metallic behavior is turned into a semiconducting one if a Kekule distortion opens a gap at the Dirac points that is larger than the chemical potential measured relative to the energy at the Dirac points. Graphene with a Kekule distortion is thus a band insulator. From the point of view of the ten-fold classification of band insulators in two-dimensional space, graphene with a Kekule distortion is topologically trivial in that it does not support gapless edge states in an open geometry that are robust to the breaking of translation invariance by an on-site real-valued potential, say. Nevertheless, graphene with a Kekule distortion supports unusual quantum numbers if the Kekule distortion is defective. For example, a point defect in the Kekule distortion binds locally a fractional value of the electron charge.

The goal of Sec. 6.7 is to study the entanglement spectrum of graphene with a Kekule distortion and show that graphene with a Kekule distortion is another example of a symmetry protected topological phase of matter.

6.7.2 Hamiltonian

We start from a honeycomb lattice $\Lambda$, whose sites are denoted with the symbol $i$. We then color the nearest-neighbor bonds of $\Lambda$ with two colors, say red and blue, as is done in Fig. 6.9(a) A pair of nearest-neighbor sites of
Figure 6.9: (a) The simplest tight-binding model for graphene with a Kekule distortion is defined by allowing spinless electrons to hop between any two nearest-neighbor sites of the honeycomb lattice with the real-valued modulated amplitudes \( t_1 \) and \( t_2 \) if a nearest-neighbor bond is colored in red or blue, respectively. The repeat unit cell of the strong and weak bonds associated to the Kekule distortion can be chosen to be made of the following three hexagons below the dashed line. The first hexagon is colored in blue and has six vertices numbered clockwise from 1 to 6. The second hexagon shares the blue bond \( \langle 12 \rangle \) with the first one. The third hexagon shares the blue bond \( \langle 23 \rangle \) to the first one. This unit cell comprised of these three hexagons is three time as large as the repeat unit cell of the honeycomb lattice with all nearest-neighbor bonds colored in black (the limiting case when \( t_1 = t_2 \)). This enlarged repeat unit cell has 6 inequivalent sites. The spanning vectors of the honeycomb lattice with the Kekule coloring of nearest-neighbor bonds are \( a_1 \) and \( a_2 \). (b) The large hexagon colored in black defines the first Brillouin zone of the triangular lattice. The small hexagon colored in blue defines the first Brillouin zone of the honeycomb lattice with the Kekule coloring of nearest-neighbor bonds. The ratio of the area of the black hexagon to the area of the blue hexagon is three to one. If the honeycomb lattice is cut along the horizontal dashed line, an armchair edge is obtained. The point denoted by \( \bullet \) at the mid-point where the dashed line intersects the nearest-neighbor bond coming out of vertex 1 below the dashed line defines the inversion center. The points \( \Gamma, M_1, M_2 \) and \( M_3 \) from the first Brillouin zone of the honeycomb lattice with the Kekule coloring of nearest-neighbor bonds are invariant (fixed) under this inversion.

To each site \( i \), we assign the anti-commuting pair \( \hat{c}^\dagger_i \) and \( \hat{c}_i \) of creation and annihilation operators, respectively. We then model graphene with a Kekule distortion on which spinless fermions hop by the Hamiltonian

\[
\hat{H}_K := \sum_{n=1,2} t_n \sum_{\langle i_n, j_n \rangle} \left( \hat{c}^\dagger_{i_n} \hat{c}_{j_n} + \text{H.c.} \right),
\]

where

\[
t_n := -t + \frac{2 \cos \left( (n - 1) \frac{2 \pi}{3} \right)}{3} \Delta_K
\]

with \( t \) and \( \Delta_K \) both real-valued. The gapless spectrum of graphene with the uniform hopping amplitude \( t \) is recovered when \( \Delta_K = 0 \).

The energy scale \( |\Delta_K| \ll |t| \) breaks the point-group symmetry of the honeycomb lattice \( \Lambda \) as is implied by the colors blue and red of inequivalent nearest-neighbor bonds in Fig. 6.9(a). The repeat unit cell of the honeycomb lattice \( \Lambda \) decorated by weak and strong bonds as is implied by the colorings in Fig. 6.9(a) can be chosen to be the three
hexagons sharing pairwise the blue bond \( \langle 12 \rangle \) and the blue bond \( \langle 23 \rangle \) in Fig. 6.9(a). The corresponding spanning vectors of the honeycomb lattice are then \( \vec{a}_1 \) and \( \vec{a}_2 \). We use the convention whereby we label the 6 sites of the blue hexagon as is done below the dashed line in Fig. 6.9(a). The site 2 belongs to one repeat unit cell. The sites 1, 3, 5 and their three images by translations belong to two repeat unit cells. The sites 4 and 6 and their four images by translations belong to three repeat unit cells. Hence, there are a total of \( 1 + 3 + 2 = 6 \) inequivalent sites in the repeat unit cell for the honeycomb lattice with the Kekule distortion. We label the site 2 from the repeat unit cell for the honeycomb lattice with the Kekule distortion by \( I \). We may then introduce the spinor

\[
\hat{\psi}^\dagger_I := \left( \hat{\psi}^\dagger_{I_1} \hat{\psi}^\dagger_{I_2} \hat{\psi}^\dagger_{I_3} \hat{\psi}^\dagger_{I_4} \hat{\psi}^\dagger_{I_5} \hat{\psi}^\dagger_{I_6} \right)
\]  

(6.198a)

obeying the fermion algebra

\[
\{ \hat{\psi}_{I_a}, \hat{\psi}^\dagger_{I'_{a'}} \} = \delta_{I,I'} \delta_{a,a'}, \\
\{ \hat{\psi}^\dagger_{I_a}, \hat{\psi}^\dagger_{I'_{a'}} \} = 0,
\]  

(6.198b)

and whose components create a spinless fermions on any one of the six inequivalent sites from the repeat unit cell \( I \) for the honeycomb lattice with the Kekule distortion. By performing a Fourier transformation to reciprocal space with momenta \( \vec{k} \) restricted to one third of the first Brillouin zone of graphene, we may rewrite Hamiltonian (6.197) as

\[
\hat{H}_K = \sum_{k \in \text{BZK}} \hat{\psi}_{k}^\dagger \mathcal{H}_k \hat{\psi}_{k},
\]

(6.199a)

where the \( 6 \times 6 \) Hermitian matrix \( \mathcal{H}_k \) is given by

\[
\mathcal{H}_k = \begin{pmatrix}
0 & t_2 & 0 & t_1 e^{-i(k_2-k_1)} & 0 & t_2 \\
t_2 & 0 & t_2 & 0 & t_1 e^{i k_1} & 0 \\
0 & t_2 & 0 & t_2 & 0 & t_1 e^{i k_2} \\
t_1 e^{i(k_2-k_1)} & 0 & t_2 & 0 & t_2 & 0 \\
0 & t_1 e^{-i k_1} & 0 & t_2 & 0 & t_2 \\
t_2 & 0 & t_1 e^{-i k_2} & 0 & t_2 & 0
\end{pmatrix}.
\]

(6.199b)

The acronym BZK stands for the reduced Brillouin zone in Fig. 6.9(b) associated to the repeat unit cell of the honeycomb lattice with a Kekule distortion. It covers one third of the area of the BZT.

### 6.7.3 Symmetries

The symmetry

\[
\mathcal{H}_{-k} = \mathcal{H}_{+k}
\]

(6.200)
implements time-reversal symmetry for spinless fermions.

The spectral symmetry

$$S^{-1} \mathcal{H}_k S = -\mathcal{H}_k,$$

(6.201a)

where

$$S := \text{diag} \ (1, -1, 1, -1, 1, -1)$$  

(6.201b)

implies the chiral (sublattice) spectral symmetry.

The symmetry

$$\mathcal{P}^{-1} \mathcal{H}_{-k} \mathcal{P} = \mathcal{H}_k,$$

(6.202a)

where

$$\mathcal{P} := \begin{pmatrix} 0 & I_3 \\ I_3 & 0 \end{pmatrix}$$

(6.202b)

implies the inversion symmetry defined with the help of Fig. 6.9(a). To define the inversion symmetry, we first draw the dashed line in Fig. 6.9(a). A cut along this dashed line defines an arm-chair boundary. We then select the intersection of the dashed line with the mid-point of the bond emerging from the site 1 of the enlarged repeat unit cell below the dashed line in Fig. 6.9(a). This mid-point, represented by a filled circle in Fig. 6.9(a), defines the inversion center. Performing an inversion about this point maps the Kekule pattern below the dashed line into the Kekule pattern above the dashed line. The two patterns are identical, hence the inversion symmetry. On the one hand, the labels in the enlarged repeat unit cell below the dashed line becomes those above the dashed line in Fig. 6.9(a) under this inversion. On the other hand, if the convention for the labels of the enlarged repeat unit cell are identical below and above the dashed line, the representation $$\mathcal{P}^{-1} \mathcal{H}_{-k} \mathcal{P} = \mathcal{H}_k$$ follows.

Observe that

$$\{S, \mathcal{P}\} = 0.$$  

(6.203)

We will make use of this anti-commutator in Sec. 6.7.5.

### 6.7.4 Partition

A slab geometry is cut from Fig. 6.9(a) by choosing two armchair edges running parallel to the $$a_1$$ direction of the two-dimensional embedding Euclidean space. Periodic boundary conditions are imposed along the $$a_1$$ direction, open ones along the $$a_2$$ direction. Hence, the momentum $$k_1$$ is a good quantum number.

This slab geometry with the choice of mixed periodic and open boundary conditions is identical to the cylindrical geometry shown in Fig. 6.6. The dashed line in Fig. 6.9(a) can be identified with the intersection of the red plane with
Figure 6.10: Energy spectrum of Hamiltonian (6.197) with armchair edges for (a) \((t_1, t_2) = (1/3, 4/3)\) and (b) \((t_1, t_2) = (5/3, 2/3)\). Entanglement spectrum with armchair entangling edges for (c) \((t_1, t_2) = (1/3, 4/3)\) and (d) \((t_1, t_2) = (5/3, 2/3)\). The dimensions of the lattice are given by \((N_1, N_2) = (128, 32)\), where \(N_i\) is the number of the repeat unit cell from Fig. 6.9(a) along the direction of the spanning vector \(a_i\) \((i = 1, 2)\) and in units for which the spanning vectors \(a_1\) and \(a_2\) are of unit length.

The dashed line in Fig. 6.9(a) will shortly be identified with an entangling boundary that is invariant under the inversion symmetry about the inversion center in Fig. 6.9(a).

We use the partition introduced in Sec. 6.5.3 with the convention that the good quantum number is \(k_1\), i.e., with \(i = 1\) in Sec. 6.5.3. The single-particle Hilbert space is the direct sum

\[
\mathcal{H} = \bigoplus_{k_1} \mathcal{H}_{k_1}.
\]  

(6.204a)

For any good momentum quantum number in the one-dimensional Brillouin zone

\[
k_1 := \frac{2\pi}{2M_1 |a_1|} n_1, \quad n_1 = 1, \ldots, 2M_1,
\]

(6.204b)

where \(N_1 = 2M_1\) is the number of enlarged unit cells along the \(a_1\) direction, the subspace \(\mathcal{H}_{k_1}\) is spanned by the orthonormal single-particle states

\[
\{ |k_1, n_2, \alpha\rangle | n_2 = 1, \ldots, 2M_2, \quad \alpha = 1, \ldots, 6 \}
\]

(6.204c)
with \( n_2 \) labeling the \( N_2 = 2M_2 \) enlarged unit cells in the direction \( \alpha_2 \) and \( \alpha = 1, \cdots, 6 \) labeling the inequivalent sites within an enlarged unit cell. The single-particle Hamiltonian \( H_{k_1} \) has matrix elements of the form given in Eq. 6.130b. The partition for any given good quantum number \( k_1 \) is then

\[
\mathcal{H}_{k_1} := \mathcal{H}_{A_2} \oplus \mathcal{H}_{B_2},
\]

where

\[
\mathcal{H}_{A_2} := \bigoplus_{n_2=1}^{M_2} \bigoplus_{\alpha=1}^{6} |k_1, n_2, \alpha \rangle \langle k_1, n_2, \alpha |
\]

and

\[
\mathcal{H}_{B_2} := \bigoplus_{n_2=M_2+1}^{2M_2} \bigoplus_{\alpha=1}^{4} |k_1, n_2, \alpha \rangle \langle k_1, n_2, \alpha |.
\]

If we denote by \( \mathcal{P} \) the inversion about the inversion center in Fig. 6.9(a) that reverses the sign of the good quantum number \( k_1 \), i.e.,

\[
\mathcal{P} k_1 = -k_1,
\]

we then have that

\[
\mathcal{P} A_2 = B_2,
\]

i.e., \( \mathcal{P} \) interchanges the physical boundaries while it leaves the entangling boundary between \( A_2 \) and \( B_2 \) invariant as a set.

### 6.7.5 Kekule with armchair edges

Both the energy and entanglement spectra are obtained by exact diagonalization with \((N_1, N_2) = (128, 32)\) and presented in Fig. 6.10 for different values of \( t_1 \) and \( t_2 \) in Eq. (6.197).

The energy spectrum is bulk-like when \( t_1 < t_2 \) as is illustrated with Fig. 6.10(a). Edge modes are not present when \( t_1 < t_2 \) in the energy spectrum, Fig. 6.10(a) being an example of this observation. For each armchair boundary, the energy spectrum supports a single pair of right- and left-moving edge states when \( t_1 > t_2 \), as is illustrated with Fig. 6.10(b). These edge states do not cross, they are gaped at the band center.

The entanglement spectrum is bulk-like when \( t_1 < t_2 \) as is illustrated with Figs. 6.10(c). Edge modes are not present when \( t_1 < t_2 \) in the entanglement spectrum, Fig. 6.10(c) being an example of this observation. For each armchair boundary, the entanglement spectrum supports a single pair of right- and left-moving edge states when \( t_1 > t_2 \), as is illustrated with Fig. 6.10(d). These edge states cross at the band center.

In the following, we shall choose \((t_1, t_2) = (5/3, 2/3)\) and study the robustness of the crossing of the edge states in
the entanglement spectrum in the presence of three symmetry-breaking perturbations. We either break time-reversal
symmetry, chiral symmetry, or inversion symmetry once at a time. Spectra obtained by exact diagonalization are
presented in Fig. 6.11 i.e., we study the spectra of

\[ \hat{H} := \hat{H}_K + \hat{H}' \]  \hspace{1cm} (6.208)

with \( \hat{H}' \) a one-body perturbation that breaks either time-reversal symmetry, chiral symmetry, or inversion symmetry.

Figure 6.11: Energy spectra are presented in the left column, entanglement spectra are presented in the right col-
umn. In both cases, the geometry is that of a slab with armchair edges as in Fig. 6.9(a) for \((t_1, t_2) = (5/3, 2/3)\)
and \((N_1, N_2) = (128, 32)\). The spectra (a) and (d) are obtained by choosing the time-reversal-breaking perturba-
tion (6.209) in Hamiltonian (6.208). The spectra (b) and (e) are obtained by choosing the chiral-symmetry-breaking
perturbation (6.210) with (6.212) in Hamiltonian (6.208). The spectra (c) and (f) are obtained by choosing the
Time-reversal symmetry breaking

We choose in Eq. (6.208) the perturbation defined by

\[
\mathcal{H}^\prime := l \begin{pmatrix}
0 & e^{i\phi} & 0 & 0 & 0 & e^{-i\phi} \\
e^{-i\phi} & 0 & e^{i\phi} & 0 & 0 & 0 \\
0 & e^{-i\phi} & 0 & e^{i\phi} & 0 & 0 \\
0 & 0 & e^{-i\phi} & 0 & e^{i\phi} & 0 \\
0 & 0 & 0 & e^{-i\phi} & 0 & e^{i\phi} \\
e^{i\phi} & 0 & 0 & 0 & e^{-i\phi} & 0
\end{pmatrix},
\]

(6.209a)

where the real number \( l \) is a uniform hopping amplitude and \( \phi \) is a uniform phase that breaks time-reversal symmetry if not equal to 0 or \( \pi \). Figures 6.11(a) and 6.11(b) give the physical energy and entanglement spectra, respectively, for \( l = 0.3, \phi = \pi/4 \).

(6.209b)

Both the chiral and the inversion symmetries are present for this perturbation that breaks time-reversal symmetry and the spectra in Figs. 6.11(a) and 6.11(d) follow. According to Fig. 6.11(a) the edge states are gaped in the energy spectrum. According to 6.11(d), the existence and location of the crossing of the edge states in the entanglement spectrum is seen to be robust to this perturbation.

Sublattice symmetry breaking

The chiral (sublattice) spectral symmetry is broken by any on-site potential. Any distribution of on-site potentials within the repeat unit cell of Fig. 6.9(a) that is unchanged under any linear combination of the spanning vectors \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \) preserves the translation symmetry of the honeycomb lattice decorated by the colors of the Kekule strong and weak bonds. Hence, we choose in Eq. (6.208) the perturbation

\[
\mathcal{H}^\prime := \text{diag} (\mu_1, \mu_2, \mu_3, \mu_4, \mu_5, \mu_6),
\]

(6.210)

where we demand that

\[
\mu_1 = \mu_4, \quad \mu_2 = \mu_5, \quad \mu_3 = \mu_6,
\]

(6.211)

breaks the chiral (sublattice) spectral symmetry for any non-vanishing value of \( \mu_n \) with \( n = 1, \cdots, 3 \) belonging to the repeat unit cell, but preserves the reduced first Brillouin zone from Fig. 6.9(b) with the inversion symmetric points \( \Gamma, M_1, M_2, \) and \( M_3 \). Since an on-site potential is represented by a real-valued matrix, \( \mathcal{H}^\prime \) does not break time-reversal
symmetry. If we use a slab geometry with two parallel armchair edges running along the $x$ axis in the embedding two-dimensional Euclidean space, we need only demand that $k_1$ is a good quantum number, i.e., invariance under translation by $\alpha_1$ only. If so, we can make the choice

$$
\mu_1 = 1/2, \quad \mu_2 = -1/4, \quad \mu_3 = \cdots = \mu_6 = 0,
$$

for the real-valued chemical potentials within the repeat unit cell. With this choice, $k_1$ is a good quantum number, the time-reversal and inversion symmetries are present, but the chiral sublattice symmetry is broken, and the spectra in Figs. 6.11(b) and 6.11(e) follow. According to Fig. 6.11(b) the edge states are gaped in the energy spectrum. According to 6.11(e), the existence and location of the crossing of the edge states in the entanglement spectrum is seen to be robust to this perturbation.

**Inversion symmetry breaking**

We choose in Eq. (6.208) the perturbation

$$
\mathcal{H}' = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
$$

(6.213a)

where the real-valued

$$
l = 0.5
$$

(6.213b)
in Figs. 6.11(c) and 6.11(f). Since this perturbation is a real-valued nearest-neighbor hopping between site 1 and 6 from the repeat unit cell of Fig. 6.9(a), time-reversal and chiral (sublattice) symmetries are present, but inversion symmetry is broken. According to Figs. 6.11(c) and 6.11(f), both the energy and entanglement spectra are gaped.

**Stability analysis of the zero modes**

The two disconnected physical boundaries in the cylindrical geometry used to do the exact diagonalization presented in Figs. 6.10 and 6.11 are interchanged by the inversion symmetry. The single entangling boundary for the cylindrical geometry considered in Figs. 6.10 and 6.11 is invariant as a set under the inversion symmetry. This difference explains why there are crossings of gapless edge states in the entanglement spectra provided $\hat{H}$ defined by
Eq. (6.197) with $t_1 > t_2$ respects the inversion (parity) symmetry $\mathcal{P}$ (and irrespectively of the presence or absence of time reversal symmetry and spectral chiral symmetry), while there are no crossing of edge states in the energy spectrum under the same assumptions.

To explain this empirical observation deduced from exact diagonalization, we assume that the existence of a pair of left- and right-moving edge states along any one of the three armchair boundaries, namely any one of the two physical armchair boundaries and the entangling armchair boundary. We consider first the case of a single physical armchair boundary and then the case of the single entangling armchair boundary. In both cases, our effective single-particle Hamiltonian for the single pair of left and right movers on an edge is given by

\[ \mathcal{H}_\text{edge} = \bigoplus_k \mathcal{H}_\text{edge}_k, \tag{6.214a} \]

where the momentum along the edge is denoted by $k$ and

\[ \mathcal{H}_\text{edge}_k = v_0 \sigma_0 + v_1 \sigma_1 + v_2 \sigma_2 + k \sigma_3 \tag{6.214b} \]

to leading order in a gradient expansion. Here, we have introduced the usual suspects, namely the $2 \times 2$ unit matrix $\sigma_0$ and the three Pauli matrices $\sigma_1, \sigma_2, \text{ and } \sigma_3$ to which we associate three energy scales through the real numbers $v_0, v_1, v_2$, and one group velocity $v_3$ that we have set to unity ($\hbar = 1$ as well), respectively.

**Energy spectrum**  The effective Hamiltonian (6.214) for a single physical armchair boundary inherits two symmetries from Hamiltonian (6.197) (the case $t_1 > t_2$ is assumed to have edge states). There is the symmetry $\mathcal{T}_\text{edge}$ under reversal of time. There is the spectral symmetry $\mathcal{S}_\text{edge}$ under multiplication by a minus sign of all the single-particle states in the position basis on one and only one of the two triangular sublattices of the honeycomb lattice. There is no inversion symmetry generated by a putative operator $\mathcal{P}_\text{edge}$ for a single physical armchair boundary. Because we have been considering spinless fermions, a representation of $\mathcal{T}_\text{edge}$ is uniquely fixed by demanding that reversal of time interchanges left and right movers while squaring to unity as an insanitary operator, i.e.,

\[ \mathcal{T}_\text{edge} := \sigma_1 K, \tag{6.215} \]

where $K$ denotes complex conjugation. Symmetry under reversal of time is the condition

\[ \mathcal{H}_{\text{edge} + k} = \sigma_1 \mathcal{H}_{\text{edge} - k}^* \sigma_1 \tag{6.216} \]
that is met for any \( v_0, v_1, \) and \( v_2 \) in Eq. (6.214). Hence, it is only the sublattice symmetry that restricts the allowed values of \( v_0, v_1, \) and \( v_2 \) in Eq. (6.214). There are two possible choices to represent \( S_{\text{edge}} \) by a unitary matrix \( S_{\text{edge}} \) such that

\[
H_{\text{edge}} k = -S_{\text{edge}} H_{\text{edge}} k S_{\text{edge}}^{-1},
\]

namely

\[
S_{\text{edge}} = \sigma_1
\]

(6.217b)

or

\[
S_{\text{edge}} = \sigma_2.
\]

(6.217c)

In both cases, the spectral symmetry (6.217) fixes the chemical potential to the value \( v_0 = 0 \). In the former case, the spectral symmetry with the generator (6.217b) fixes \( v_1 = 0 \) but leaves \( v_2 \) arbitrary so that a gap opens up as soon as \( v_2 \neq 0 \) in the energy spectrum of the edge states. In the latter case, the spectral symmetry with the generator (6.217c) fixes \( v_2 = 0 \) but leaves \( v_1 \) arbitrary so that a gap opens up as soon as \( v_1 \neq 0 \) in the energy spectrum of the edge states.

**Entanglement spectrum** We now assume that the single pair of left and right movers propagating along the entangling boundary is governed by the effective

\[
Q_{\text{edge}} A k \equiv H_{\text{edge}} k
\]

(6.218)

with \( H_{\text{edge}} k \) defined in Eq. (6.214). The symmetries obeyed by \( Q_{\text{edge}} A k \) are

\[
Q_{\text{edge}} A + k = T_{\text{edge}} Q_{\text{edge}} A - k T_{\text{edge}}^{-1},
\]

(6.219a)

\[
Q_{\text{edge}} A k^\dagger = -S_{\text{edge}} Q_{\text{edge}} A k S_{\text{edge}}^{-1},
\]

(6.219b)

\[
Q_{\text{edge}} A + k = -\Gamma_{P_{\text{edge}}} Q_{\text{edge}} A - k \Gamma_{P_{\text{edge}}}^{-1},
\]

(6.219c)

[Recall Eq. (6.53b)]. Needed is a representation of the unitary generator \( \Gamma_{P_{\text{edge}}} \) for inversion on the entangling boundary. Since

\[
k \sigma_3 = -\sigma_\mu (-k \sigma_3) \sigma_\mu
\]

(6.220)

for both \( \mu = 0 \) or \( \mu = 3 \), there seems to be an ambiguity when defining \( \Gamma_{P_{\text{edge}}} \). On the one hand, choosing

\[
\Gamma_{P_{\text{edge}}} = \sigma_0
\]

(6.221a)
implies that $\Gamma_{p_{\text{edge}}}$ commutes with either choices (6.217b) or (6.217c). On the other hand, choosing
\[
\Gamma_{p_{\text{edge}}} = \sigma_3
\] (6.221b)
implies that $\Gamma_{p_{\text{edge}}}$ anti-commutes with either choices (6.217b) or (6.217c). Now, it is only when $\Gamma_{p_{\text{edge}}}$ commutes with $S_{\text{edge}}$ that inversion symmetry protects the crossing of the pair of edge states at the band center by fixing $v_0 = v_1 = v_2 = 0$ irrespectively of whether sublattice symmetry holds or not! The ambiguity in choosing between the representations (6.221a) and (6.221b) is spurious, however. We must choose the representation (6.221a) as we now demonstrate.

We are now going to show that irrespective of the choice made to represent $S_{\text{edge}}$, we must choose to represent $P_{\text{edge}}$ such that
\[
[S_{\text{edge}}, \Gamma_{p_{\text{edge}}}] = 0.
\] (6.222)
To this end, we use the fact that the chiral transformation representing the spectral sublattice symmetry and that representing the inversion symmetry in the bulk, recall Eq. (6.201) and (6.202), anti-commute according to Eq. (6.203).

In the presence of inversion symmetry, there is a spectral symmetry $\Gamma_{\varphi}$ in the entanglement spectrum. This spectral symmetry was defined by $\Gamma_{\varphi} = C_{ABk} P$ in Eq. (6.46d) (we are using the conventions of Sec. 6.2.1 for the choice of the fonts of the symmetry generators). In the presence of the spectral symmetry
\[
S Q_{A_k} S^{-1} = -Q_{A_k}
\] (6.223)
and
\[
S C_{ABk} S^{-1} = -C_{ABk}
\] (6.224)
with the anti-commutator $\{S, P\} = 0$ in agreement with Eq. (6.203). We then have
\[
[S, \Gamma_{\varphi}] = [S, C_{ABk} P] = \{S, C_{ABk}\} P - C_{ABk} \{S, P\} = 0.
\] (6.225)

We have constructed the explicit representations of $S$ and $\Gamma_{\varphi}$ obtained after exact diagonalization of Eq. (6.208) and verified that Eq. (6.225) holds.
Figure 6.12: (a) The nearest-neighbor bonds of the honeycomb lattice are colored in red, blue, and green as depicted. The colors red, blue, and green correspond to the values $t_1$, $t_2$, and $t_3$ taken by the nearest-neighbor hopping amplitudes for spinless fermions hopping on the honeycomb lattice with Hamiltonian (6.226), respectively. The repeat unit cell with its spanning vectors $a_1$ and $a_2$ was defined in Fig. 6.9(a). An armchair entangling edge is obtained by opening the honeycomb lattice through the dashed line. (b) The cylindrical geometry with the two armchair edges differing by their colors is selected by imposing periodic boundary conditions along the $a_1$ direction and open ones along the $a_2$ direction. The top armchair edge denoted by a red ellipse has fermions hopping along it with the consecutive hopping amplitudes $t_1$, $t_2$, $t_3$, and $t_2$. The bottom armchair edge denoted by the blue ellipse has fermions hopping along it with the consecutive hopping amplitudes $t_1$, $t_3$, $t_2$, and $t_3$. [Note that these are not the armchair boundaries shown in panel (a).]

6.7.6 Rotated Kekule with armchair edges

The honeycomb lattice is unchanged under rotations by $\pi/3$ about the center of an elementary hexagon. The Kekule order breaks this point-group symmetry down to rotations by $2\pi/3$ about the center of an elementary hexagon. This pattern of symmetry breaking is that of $C_6 \rightarrow C_3$, where $C_n$ is the $n$-fold rotation symmetry group. Rotations by arbitrary angles about a point in a plane form a group, the Abelian group $U(1)$. This suggests a connection between the Kekule order parameter and the spontaneous breaking of an internal symmetry group $U(1)$. This connection becomes precise in the approximation by which the spectrum of graphene is linearized about the Dirac points. The actions of rotations about the center of an hexagon in graphene involve, in the Dirac approximation, a mixing of the components of the Dirac spinors through the action of one of the Dirac matrices denoted $\gamma_5$. In the terminology of high-energy physics, $\gamma_5$ is associated to a pseudoscalar charge called the axial charge. For graphene, this pseudoscalar charge is the difference in the local density of electrons associated to the two valleys of graphene.

In the Dirac limit, the pattern of symmetry breaking induced by a Kekule distortion becomes the spontaneous breaking of a continuous $U(1)$ symmetry generated by the axial gauge charge.

The Kekule distortion can support a point defect at which three Kekule distortions differing pairwise by a global
Figure 6.13: (a) Energy spectrum with two armchair edges in the cylindrical geometry of Fig. 6.12(b). (b) Entanglement spectrum with two entangling armchair boundaries in a toroidal geometry. The energy scales are $\Delta_0 = 1$ and $t = -1$. The axial phase is $\alpha \approx 5.927$. The lattice size is $(N_1, N_2) = (128, 32)$. The number of unit cells along $\alpha_i$ is $N_i$ for $i = 1, 2$.

axial phase of either $2\pi/3$ or $4\pi/3$ (mod $2\pi$) meet. With open boundary conditions, such a point defect was shown to support two localized zero modes. There is one zero mode localized around the point defect. There is one zero mode localized somewhere on the boundary. The location on the boundary of the latter zero mode depends on the value taken by the global axial phase of the defective Kekule distortion.

Our purpose is to study the influence of the choice made for the global axial phase of a uniform Kekule distortion on the spectrum of the Kekule Hamiltonian with armchair open boundary conditions.

Rotated Kekule distortion

To parametrize a global rotation of a Kekule distortion, we define

$$\hat{H}_K(\alpha) := \sum_{n=1,2,3} t_n(\alpha) \sum_{\langle i,j \rangle_n} \left( \hat{c}_i^n \hat{c}_{j,n}^\dagger + \text{H.c.} \right),$$  \hspace{1cm} (6.226a)

where

$$t_n(\alpha) := -t + \frac{1}{3} \left( \Delta_K(\alpha) e^{i(n-1)2\pi/3} + \Delta_K^*(\alpha) e^{-i(n-1)2\pi/3} \right),$$ \hspace{1cm} (6.226b)

and

$$\Delta_K(\alpha) := \Delta_{K0} e^{+i\alpha}. \hspace{1cm} (6.226c)$$

Here, $t$ is real-valued and the Kekule distortion has the amplitude $\Delta_{K0} \geq 0$ and global axial phase $0 \leq \alpha < 2\pi$. Moreover, a pair of nearest-neighbor sites of the honeycomb lattice is denoted by $\langle i,j \rangle$ if they are connected by a bond colored in red ($i = 1$), blue ($i = 2$), and green ($i = 3$), respectively as is depicted in Fig. 6.12(a).
On a torus, two-dimensional momentum $k \equiv (k_1, k_2)$ is a good quantum number and the single-particle Hamiltonian with a rotated Kekule distortion becomes (the $\alpha$ dependence is implicit)

$$H_k = \begin{pmatrix}
0 & t_2 & 0 & t_1 e^{-i(k_2-k_1)} & 0 & t_3 \\
t_2 & 0 & t_3 & 0 & t_1 e^{+i k_1} & 0 \\
0 & t_3 & 0 & t_2 & 0 & t_1 e^{+i k_2} \\
0 & t_1 e^{+i (k_2-k_1)} & 0 & t_2 & 0 & t_3 \\
0 & t_1 e^{-i k_1} & 0 & t_3 & 0 & t_2 \\
t_3 & 0 & t_1 e^{-i k_2} & 0 & t_2 & 0
\end{pmatrix} \quad (6.227)$$

For vanishing global axial phase, Hamiltonian (6.227) reduces to Hamiltonian (6.199b). Hamiltonian (6.227) is invariant under the same operation for time-reversal as was the case for Hamiltonian (6.199b). The spectrum of Hamiltonian (6.227) is invariant under the same chiral (sublattice) operation as was the case for Hamiltonian (6.199b). Hamiltonian (6.227) breaks the inversion symmetry enjoyed by Hamiltonian (6.199b) for any $\alpha \neq 0 \text{ mod } 2\pi$. This can be seen by inspection of the armchair boundaries in Fig. 6.12(a) and is indicated in Fig. 6.12(b) by the distinct colors used to denote the two edges if a cylindrical geometry is selected by the choice of boundary conditions with the direction $a_2$ the open direction.

**Spectra for rotated Kekule**

The energy spectrum as a function of the good momentum quantum number $k_1$ is computed by diagonalizing the Hamiltonian (6.226) in the cylindrical geometry of Fig. 6.12(b). For any $\alpha \neq 0 \text{ modulo } 2\pi$, inversion symmetry is broken so that the quantum dynamics on the opposite edges of the cylinder in Fig. 6.12(b) differ. Remarkably, at a critical value of the axial angle $\alpha_c$, the gap for the single pair of left- and right-movers on one of the edges closes, while it does not for the single pair of left- and right-movers from the other edge. This property of the energy spectrum of the rotated Kekule distortion is illustrated in Fig. 6.13(a). The critical value of the axial angle $\alpha_c$ is $\alpha_c \approx 5.927$ when $(\Delta_{K0}, t) = (1, -1)$, as we now show. To this end, we use the $4 \times 4$ Hamiltonians

$$H_{\text{edge}}^{\text{top} k_1}(\alpha) := \begin{pmatrix}
0 & t_1(\alpha) & 0 & t_2(\alpha) e^{+i k_1} \\
t_1(\alpha) & 0 & t_2(\alpha) & 0 \\
0 & t_2(\alpha) & 0 & t_3(\alpha) \\
t_2(\alpha) e^{-i k_1} & 0 & t_3(\alpha) & 0
\end{pmatrix} \quad (6.228)$$
and

\[
\mathcal{H}_{\text{edge}}^{\bot k_1}(\alpha) := \begin{pmatrix}
0 & t_1(\alpha) & 0 & t_3(\alpha) e^{+ik_1} \\
0 & 0 & t_3(\alpha) & 0 \\
t_3(\alpha) e^{-ik_1} & 0 & t_2(\alpha) & 0 \\
t_1(\alpha) & 0 & 0 & t_3(\alpha)
\end{pmatrix}
\] (6.229)

to model hopping restricted to the top and bottom armchair boundaries defined in Fig. 6.14, respectively. For the top armchair edge, we are using four orbitals per repeat unit cell with the conventions that orbital 1 hops to orbital 2 with the amplitude \( t_1(\alpha) \), orbital 2 hops to orbital 3 with the amplitude \( t_2(\alpha) \), orbital 3 hops to orbital 4 with the amplitude \( t_3(\alpha) \), and orbital 4 hops to orbital 1 in the neighboring repeat unit cell with the amplitude \( t_2(\alpha) \). For the bottom armchair edge, we are using the conventions that follow from those for the top armchair edge obtained by exchanging \( t_2(\alpha) \) and \( t_3(\alpha) \). Eigenstates of Hamiltonian \( \mathcal{H}_{\text{edge}}^{\text{top} k_1}(\alpha) \) at \( k_1 = 0 \) with zero energy eigenvalue satisfy

\[
\det \left[ \mathcal{H}_{\text{edge}}^{\text{top} k_1}(\alpha) \right] = 0.
\]

This condition gives \( \alpha_c \approx 5.927 \) when \( (\Delta_{K0}, t) = (1, -1) \) for the critical axial angle.

We have also calculated the entanglement spectrum using the same partition as the one used in Sec. 6.7.4, with the proviso that we are now using the dashed line shown in Fig. 6.12(a). To avoid contamination in the entanglement spectrum arising from the gap closing along one of the physical edges when \( \alpha = \alpha_c \), we choose to impose full periodic boundary conditions, i.e., the geometry of a torus. We expect no closing of the entanglement spectrum because of the breaking of inversion symmetry by any \( \alpha \neq 0 \) modulo \( 2\pi \) and indeed, this is what is observed from exact diagonalization and illustrated with the help of Fig. 6.13(b).

### 6.7.7 Kekule with zigzag edges

**Hamiltonian**

The energy spectrum of semi-infinite graphene modeled by a single nearest-neighbor hopping amplitude on the honeycomb lattice with a zigzag edge shows flat (dispersionless) bands connecting the two Dirac points. These zero-energy flat bands are protected by chiral symmetry, see Ref. 196. These flat bands can become dispersive by tuning on when perturbed by a one-body potential that breaks the inversion symmetry, as demonstrated in Ref. 197. We consider the energy and entanglement spectra of graphene with a Kekule distortion in the presence of physical and entangling zigzag edges. The repeat unit cell and the spanning vectors are defined in Fig 6.14. With the conventions of Fig 6.14, the BZ and four inversion symmetric momenta are identical to the BZ and four inversion symmetric momenta from Fig 6.9(b) if we impose periodic boundary conditions.
Figure 6.14: The nearest-neighbor bonds of the honeycomb lattice are colored in red and blue as depicted. The colors red and blue correspond to the values $t_1$ and $t_2$ taken by the nearest-neighbor hopping amplitudes for spinless fermions hopping on the honeycomb lattice with Hamiltonian (6.230), respectively. A Kekule distortion follows from choosing $t_1 \neq t_2$. A physical zigzag edge is constructed from cutting through the dashed line. The dashed line also defines a zigzag entangling edge. The symbol • denotes an inversion center. One repeat unit cell contains three hexagons defined as follows. The first hexagon from the repeat unit cell has two sites numbered 1 and 2, whereby site 1 is connected by a blue bond to site 2. The second hexagon from the repeat unit cell has three sites numbered 2, 3, and 4, whereby site 2 is connected by a blue bond to site 3, while site 3 is connected by a red bond to site 4. The third hexagon from the repeat unit cell has all six edges colored in blue with the vertices numbered 4, 5, and 6. The spanning vectors corresponding to this unit cell are $\mathbf{a}_1$ and $\mathbf{a}_2$. The image of the repeat unit cell under inversion about the point • is has its three hexagons labeled with the numbers 1 to 6 written upside down.

The single particle Hamiltonian in momentum space is

$$
H_{\text{zig}} k =
\begin{pmatrix}
0 & t_2 & 0 & t_2 e^{-ik_2} & 0 & t_1 e^{-ik_1} \\
t_2 & 0 & t_2 & 0 & t_1 e^{i(k_2-k_1)} & 0 \\
0 & t_2 & 0 & t_1 & 0 & t_2 e^{-ik_2} \\
t_2 e^{ik_2} & 0 & t_1 & 0 & t_2 & 0 \\
0 & t_1 e^{-i(k_2-k_1)} & 0 & t_2 & 0 & t_2 \\
t_1 e^{ik_1} & 0 & t_2 e^{ik_2} & 0 & t_2 & 0
\end{pmatrix}
$$

(6.230)

**Symmetries**

The symmetry

$$
H_{\text{zig}}^* k = H_{\text{zig}} k
$$

(6.231)

implements time-reversal symmetry for spinless fermions.

The spectral symmetry

$$
S^{-1} H_{\text{zig}} k S = -H_{\text{zig}} k
$$

(6.232a)
Figure 6.15: Energy spectra of $H_{\text{zig},k_1}$ in Eq. (6.235) with zigzag edges in a cylinder geometry for (a) $(t_1, t_2) = (1/3, 4/3)$ and (b) $(t_1, t_2) = (5/3, 2/3)$. Entanglement spectra of $H_{\text{zig},k_1}$ in Eq. (6.235) with zigzag entangling edges in a torus geometry for (c) $(t_1, t_2) = (1/3, 4/3)$ and (d) $(t_1, t_2) = (5/3, 2/3)$. The dimensions of the lattice are given by $(N_1, N_2) = (128, 32)$, where $N_i$ is the number of the repeat unit cell from Fig. 6.14 along the direction of the spanning vector $a_i$ ($i = 1, 2$) and in units for which the spanning vectors $a_1$ and $a_2$ are of unit length.

where

$$S := \text{diag} \ (1, -1, 1, -1, 1, -1)$$

(6.232b)

implements the chiral (sublattice) spectral symmetry. The symmetry

$$\mathcal{P}_z^{-1} H_{\text{zig}} - k \mathcal{P}_{\text{zig}} = H_{\text{zig}} + k,$$

(6.233a)

where

$$\mathcal{P}_{\text{zig}} := \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

(6.233b)

implements the inversion symmetry defined with the help of Fig. 6.14. To define the inversion symmetry, we first draw

136
the dashed line in Fig. 6.14. A cut along this dashed line defines a zigzag boundary. We then select the intersection of the dashed line with the mid-point of a hexagon in Fig. 6.14. This mid-point, represented by a filled circle in Fig. 6.14, defines the inversion center. Performing an inversion about this point maps the Kekule pattern on the right of the dashed line into the Kekule pattern on the left of the dashed line. The two patterns are identical, hence the inversion symmetry. On the one hand, the labels in the enlarged repeat unit cell on the right of the dashed line becomes those on the left the dashed line in Fig. 6.14 under this inversion. On the other hand, if the convention for the labels of the enlarged repeat unit cell are identical on the right and left of the dashed line, the representation (6.233) follows.

Observe that
\[
\{S, P_{\text{zig}}\} = 0.
\] (6.234)

**Partition**

The partition is defined with respect to the dashed line in Fig. 6.15 as was done in Sec. 6.7.4.

**Hamiltonian and entanglement spectra**

Let
\[
H_{k_1} := H_{\text{zig}} k_1 + H',
\] (6.235)

where \(H'\) is a one-body perturbation that breaks either the chiral symmetry, the inversion symmetry, or both, and we have imposed periodic boundary conditions along the \(a_1\) direction from Fig. 6.15 so that \(k_1\) is a good quantum number. Open boundary conditions are imposed along the \(a_2\) direction from Fig. 6.15 when computing energy spectra. Periodic boundary conditions are imposed along the \(a_2\) direction from Fig. 6.15 when computing entanglement spectra in order to avoid a spectral contamination of the entanglement boundary states arising from the zero modes from the physical boundaries.

We have studied by exact diagonalization both the energy and entanglement spectra of Hamiltonian (6.235) in a cylinder and torus geometry, respectively.

In the absence of the perturbation \(H'\), non-dispersing edge states at zero energy are present for any Kekule distortion, i.e., as soon as \(t_1 \neq t_2\), as is illustrated in Figs. 6.15(a) and 6.15(b). Non-dispersing zero modes localized on the entangling boundary are also found in the entanglement spectrum for any Kekule distortion, i.e., as soon as \(t_1 \neq t_2\), as is illustrated in in Figs. 6.15(c) and 6.15(d).

In the following, the number of repeat unit cells are \((N_1, N_2) = (128, 32)\) and we set \((t_1, t_2) = (5/3, 2/3)\) when studying the robustness of the flat (entangling) edge states in the presence of three distinct \(H'\).
**Inversion symmetry breaking**  The inversion-symmetry-breaking perturbation is chosen in Eq. 6.235 to be

\[
H' := \begin{pmatrix}
0 & v'_1 e^{+i k_1} & 0 & 0 & 0 \\
v'_1 e^{-i k_1} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{pmatrix},
\]  

(6.236)

where \( v'_1 = 0.5 \). The flat bands when \( v'_1 = 0.5 \) are robust in both the energy and the entanglement spectra under this inversion-symmetry-breaking but chiral-symmetry-preserving perturbation as is shown in Fig. 6.16(a) and 6.16(d), respectively.

**Chiral symmetry breaking**  The chiral-symmetry-breaking perturbation is chosen in Eq. 6.235 to be

\[
H' := \text{diag} \left( o_1, o_2, o_3, o_4, o_5, o_6 \right),
\]  

(6.237)

where \( o_1 = -0.13, o_2 = 0.2, \) and \( o_3 = 0.3 \). The flat bands when \( o_1 = o_2 = o_3 = 0 \) are shifted away from zero energy in the energy spectrum shown in Fig. 6.16(b). However, the flat bands when \( o_1 = o_2 = o_3 = 0 \) are unchanged by \( H' \) in the entanglement spectrum shown in Fig. 6.16(e).

**Chiral symmetry and inversion symmetry breaking**  The inversion-symmetry-breaking and chiral-symmetry-breaking perturbation is chosen in Eq. 6.235 to be

\[
H' := \text{diag} \left( o_1, o_2, o_3, o_4, o_5, o_6 \right),
\]  

(6.238)

where \( (o_1, o_2, o_3, o_4, o_5, o_6) = (0, 0.1, 0.2, 0.3, 0.2, 0.1) \) in Figs. 6.16(c) and 6.16(f). This chiral-symmetry-breaking and inversion-symmetry-breaking perturbation gaps out the flat bands when \( (o_1, o_2, o_3, o_4, o_5, o_6) = (0, 0, 0, 0, 0) \) both in the energy and entanglement spectra shown in Fig. 6.16(c) and 6.16(f), respectively.

**Stability analysis of the zero modes**

We have observed numerically that flat bands in \( \sigma(H'_{zg k_1}) \) and \( \sigma(Q_{A k_1}) \) can only be gaped when both the chiral and inversion symmetries are broken. To understand this result, we proceed in two steps.

First, we observe numerically that (i) there is one edge state per momentum and per edge (with a wavefunction
Figure 6.16: Energy spectra of $H_{k_1}$ in Eq. (6.235) with zigzag edges in a cylindrical geometry are presented in the left column. Entanglement spectra of $H_{k_1}$ in Eq. (6.235) with zigzag entangling edges in a torus geometry are presented in the right column. In both cases, we set $(t_1, t_2) = (5/3, 2/3)$ and $(N_1, N_2) = (128, 32)$. The spectra (a) and (d) are obtained by choosing the inversion-breaking perturbation (6.236) in Hamiltonian (6.235). There are mid-gap flat bands that are two-fold degenerate. The spectra (b) and (e) are obtained by choosing the chiral-symmetry-breaking perturbation (6.237) in Hamiltonian (6.235). The flat bands remain two-fold degenerate but are shifted away from zero energy in panel (b). The spectra (c) and (f) are obtained by choosing both the inversion-symmetry-breaking and chiral-symmetry-breaking perturbation (6.238) to Hamiltonian (6.235). The two-fold degeneracy of the flat bands is lifted and all flat bands are shifted away from the eigenvalue zero in panels (c) and (f).

Properties (i) and (ii) imply that the effective edge theory on an isolated single zigzag edge of the Hamiltonian $H_{\text{zig} \ k_1}$ is the momentum-resolved $1 \times 1$ matrix

$$H_{\text{edge} \ k_1} = m_{\text{energy}} \in \mathbb{R},$$

(6.239a)

whereas that on an isolated single zigzag edge of the entangling operator $Q_{A \ k_1}$ is the momentum-resolved $1 \times 1$ matrix

$$Q_{\text{edge} \ A \ k_1} = m_{\text{entanglement}} \in \mathbb{R}.$$

(6.239b)

Chiral symmetry imposes the constraints

$$S_{\text{edge}}^{-1} H_{\text{edge} \ k_1} S_{\text{edge}} = -H_{\text{edge} \ k_1},$$

(6.240a)
and
\[ S_{\text{edge}}^{-1} Q_{\text{edge}} A_{k_1} S_{\text{edge}} = -Q_{\text{edge}} A_{k_1}, \]  
(6.240b)

These constraints can only be met if
\[ \mathcal{H}_{\text{edge} k_1} = 0 \]  
(6.241a)

and
\[ Q_{\text{edge}} A_{k_1} = 0. \]  
(6.241b)

Thus, it is the spectral chiral symmetry (6.232) that explains the presence of the mid-gap flat bands in panels (a) and (d) from Fig. 6.16. The breaking of the spectral chiral symmetry (6.232) by the perturbation (6.237) in panels (b) and (e) is manifest in the fact that the flat bands in panel (b) are not to be found anymore at the energy eigenvalue zero. The fact that the flat bands in panel (e) remains at the eigenvalue zero must be attributed to another protecting symmetry.

Second, in the presence of the inversion symmetry (6.233), there exists the operator \( \Gamma_{\mathcal{P}_{\text{zig}}} \) such that [recall Eq. (6.53)]
\[ \Gamma_{\mathcal{P}_{\text{zig}}} Q_{\text{edge}} A_{k_1} = -Q_{\text{edge}} A_{k_1} \Gamma_{\mathcal{P}_{\text{zig}}}. \]  
(6.242)

This effective chiral symmetry of the entanglement spectrum is the reason why panel (e) from Fig. 6.16 displays a two-fold degenerate flat band at the eigenvalue zero, whereas the two-fold degenerate flat band in panel (b) from Fig. 6.16 is at a non-vanishing energy eigenvalue that is determined by the amount of breaking of the spectral chiral symmetry by the perturbation (6.237). As soon as the inversion symmetry and the spectral chiral symmetry are simultaneously broken, as it is in panels (c) and (f) from Fig. 6.16 by the perturbation (6.238), the flat bands are to be found at non-vanishing distances from the eigenvalue zero in both the energy and the entanglement spectra, while their degeneracy has been lifted.

### 6.7.8 Counting the mid-gap states protected by inversion symmetry

The stability analysis of the zero modes that we have conducted so far relied on the number of edges states determined numerically before the introduction of perturbations. However, this number of zero modes can be determined analytically as follows.

It was shown in Ref. [158] that a two-dimensional topological band insulator protected by inversion symmetry is characterized by the number of zero modes \( n_{\text{zero}}^{A,k_i,k_i^*} \) in the entanglement spectrum \( \sigma(Q_{A,k_i}) \) defined with periodic boundary conditions (torus geometry). Here, we recall that the entangling boundary defined by the partition \( A \) is characterized by the good momentum quantum number \( k_i \) where \( i = 1, 2 \) while \( i + 1 \) is defined modulo 2 and that \( k^* = (k_1^*, k_2^*) \) is any momentum from the Brillouin zone that is unchanged modulo the addition of a momentum from...
the reciprocal lattice with the two spanning vectors $Q_1$ and $Q_2$ under the operation of inversion. In turn, it was shown in Refs. [158] and [157] that

$$n^\text{zero}_{A,k_i,k_j} = 2 \left| n_{k^*} - n_{k^*+(Q_{i+1}/2)} \right|,$$

(6.243)

where $n_{k^*}$ is the number of occupied Bloch eigenstates at the inversion symmetric momentum $k^*$ of the single-particle Hamiltonian (defined with periodic boundary conditions) that are simultaneous eigenstates of the inversion operator. The counting formula (6.243) is here meaningful because (i) $k^*$ and $k^* + (Q_{i+1}/2)$ are both invariant under the operation of inversion modulo the addition of a reciprocal momentum and (ii) it is possible to simultaneously diagonalize the Bloch Hamiltonian at any inversion symmetric momentum point and the operator that represents the operation of inversion. Equation (6.243) is remarkable in that it relates a property from the entangling boundary, the integer $n^\text{zero}_{A,k_i,k_j}$, to a property of the bulk, the integer $n_{k^*} - n_{k^*+(Q_{i+1}/2)}$. Equation (6.243) is thus an example of a bulk-boundary correspondence. We choose the Fermi energy to be zero and apply Eq. (6.243) to graphene with a Kekule distortion.

Graphene with a Kekule distortion, in its simplest incarnation, has six bands that are related by the chiral operation consisting in changing the sign of the wavefunction on all the sites of one of the two triangular sublattices of the honeycomb lattice. This spectrum of graphene with a Kekule distortion is thus chiral symmetric. Hence, there are three occupied bands with strictly negative energy eigenvalues when the Fermi energy is vanishing, i.e., coincides with the mid-gap single-particle energy.

We are going to apply the counting formula (6.243) to graphene with the Kekule distortion and at a vanishing Fermi energy by choosing the inversion point to be either along an armchair cut as in Fig. 6.9 or along a zigzag cut as in Fig. 6.12. The inversion symmetric momenta from the Brillouin zone are then

$$k^* \in \{(0,0)^T, (\pi,0)^T, (0,\pi)^T, (\pi,\pi)^T\},$$

(6.244)

where we have chosen units such that the spanning vectors of the reciprocal lattice are $Q_1 = (2\pi,0)^T$ and $Q_2 = (0,2\pi)^T$.

**Armchair cut** For the armchair case with Hamiltonian (6.199b), we assign to each of the four inversion-symmetric momenta (6.244) the row vector consisting of the three parities under the operation of inversion of the three occupied
Bloch states according to

\[
\begin{align*}
\Gamma(k_1 = 0, k_2 = 0) : & \quad (-, -, -), \\
M_1(k_1 = \pi, k_2 = 0) : & \quad (+, -, +), \\
M_2(k_1 = 0, k_2 = \pi) : & \quad (+, -, +), \\
M_3(k_1 = \pi, k_2 = \pi) : & \quad (+, -, +).
\end{align*}
\]

Hence, the number \(6.243\) of zero modes is four (two per entangling edge in a torus geometry) at \(k_1 = 0\) and is zero at \(k_1 = \pi\) in agreement with our numerics.

**Zigzag cut**  For the zigzag case with Hamiltonian \(6.230\), we assign to each of the four inversion-symmetric momenta \(6.244\) the row vector consisting of the three parities under the operation of inversion of the three occupied Bloch states according to

\[
\begin{align*}
\Gamma(k_1 = 0, k_2 = 0) : & \quad (-, +, +), \\
M_1(k_1 = \pi, k_2 = 0) : & \quad (-, -, +), \\
M_2(k_1 = 0, k_2 = \pi) : & \quad (+, -, -), \\
M_3(k_1 = \pi, k_2 = \pi) : & \quad (+, -, +).
\end{align*}
\]

Hence, the number \(6.243\) of zero modes is two (one per entangling edge in a torus geometry) at both \(k_1 = 0\) and \(k_1 = \pi\) in agreement with our numerics.

## 6.8 Conclusion

The main focus of this chapter has been on fermionic single-particle local Hamiltonians obeying three conditions. First, the many-body ground state is non-degenerate and incompressible if periodic boundary conditions are chosen. In short, the ground state is that of a band insulator. Second, point-group symmetries generated by non-local transformations such as a reflection or inversion must hold. Third, certain boundary conditions that are compatible with the point-group symmetries must be imposed on the entanglement spectrum through the choice of entangling boundaries. We have then constructed several examples of model Hamiltonians obeying all three conditions in one- and two-dimensional space with the following two properties. First, each model supports gapless boundary states in the entanglement spectrum that are localized on an isolated entangling boundary, even though no gapless boundary states can be found in the energy spectrum on an isolated physical boundary. Second, the stability under (one-body) perturbations of the gapless boundary states in the entanglement spectrum is guaranteed by the point-group symmetries.
Common to all these examples is the fact that the non-local point-group symmetries in the energy spectrum become local spectral symmetries in the entanglement spectrum, as we have shown. The existence of these symmetry-protected gapless boundary states in the entanglement spectrum is a signature of a topological character, for it is dependent on the choice of boundary conditions. Whereas counting them relies explicitly on the point-group symmetries, as in Eq. (6.243) say, [157, 158] our main results (6.46) and (6.53) offer a complementary understanding to their stability.
Chapter 7

Conclusion and outlook

The main focus of this thesis is to explore the physical nature and implications of gapless topological phases. We demonstrate a classification of topological stable Fermi surfaces in semimetals and nodal superconductors by use of K-theory arguments and a dimensional reduction procedure from higher-dimensional topological insulators and superconductors. In the presence of discrete symmetries, i.e., time-reversal symmetry and/or particle-hole symmetry, non-trivial topological features emerge in these gapless topological phases. The appearance of the protected zero-energy edge (surface) states on the boundary has a direct link to the topological invariants characterizing Fermi surfaces in bulk—a generalized bulk-boundary correspondence. In addition to the protected zero-energy edge (surface) states, we observe various types of vortex states in nodal NCSs depend on the point-group symmetry and the geometry of the line node.\footnote{The geometry of the Fermi surfaces means the orientations and shapes of the Fermi surfaces.} This observation indicates that topological gapless phases are more complex and have richer topological properties than the topological gapped phases. Here, we would like to highlight two remarks:

1. Various types of Fermi surfaces give the complexity and richness in gapless phases (see Figs. 3.3 and 4.1).

2. The changes of geometry of Fermi surfaces undergo a Lifshitz transition that can lead to different types of surface and vortex states in the system (see Figs. 4.1 and 4.4).

To conclude, the geometry of Fermi surfaces has a direct link to the topological properties of gapless phases. At the end of the thesis, we would like to point out some interesting ongoing researches and future directions of the field of topological gapless phases.

1. Mirror symmetry protected gapless phases have been studied recently in Ref \[137\]. We can extend this idea to $n$-fold rotational symmetry protected Fermi points/lines.

2. Anomalous electrical transport in Weyl semimetals have been extensively studies in Refs. \[49\][52]. It will be interesting to study the thermal and thermoelectric transport of topological nodal superconductors. Specifically, we can calculate the thermal current of the nodal NCSs in the presence of the vortices. A promising outcome of this calculation is that the thermal current will be induced by vortices and will propagate along the vortex.
lines. This phenomenon is a realization of a quantum anomaly in nodal superconductors that is an analogy of magnetic field induced current in topological semimetals.

3. Another interesting aspect is to study the effects of interactions and disorder on topological gapless phases. First, we should analyze the stability of Fermi surfaces in the presence of interactions and disorder. Rather, exotic surface states with fractionalized excitations can emerge on fully gapped topological phases in the presence of strong interactions. And the disorder was also shown to play an essential role by enhancing the interactions on the surface of gapped superconductors. We shall also explore these effects in the gapless phases.
Appendix A

A.1 Topological invariants

A.1.1 Berry connection, curvature, flux, and Chern number

For a given single particle Hamiltonian \( H(k) \) in momentum space with the eigenstate \( |u_a(k)\rangle \) and energy \( E_a(k) \), the non-Abelian Berry connection is defined by

\[
A^{ab}(k) = A^{ab}_\mu(k) dk_\mu = \langle u^-_a(k) | du^b_\mu(k) \rangle, \quad \mu = 1, \cdots, d, \quad a, b = 1, \cdots, N_-,
\]

where \( N_- \) is the highest occupied band. By definition, the Berry curvature is

\[
F^{ab}(k) = dA^{ab} + (A^2)^{ab} = \frac{1}{2} F^{ab}_{\mu\nu} dk_\mu \wedge dk_\nu.
\]

The Berry flux is defined as

\[
B_\mu = \frac{1}{2} \epsilon_{\mu\nu\lambda} Tr[F_{\nu\lambda}].
\]

The Chern number is defined as

\[
C = \frac{i}{2\pi} \int_S dS \cdot B,
\]

where \( S \) is a surface. The Chern number is an integer value if \( S \) is a closed manifold — a \( \mathbb{Z} \) topological invariant.

A.1.2 Systems with chiral symmetry

We start from a general lattice Hamiltonian \( H = \sum_k \Psi_k^\dagger H(k) \Psi_k \) describing time-reversal invariant superconductors with \( N \) bands and two spin degrees of freedom. The following derivation of \( \mathbb{Z} \) topological invariants (Sec. A.1.2)
is applicable to any Hamiltonian $H(k)$ with chiral symmetry, i.e., any $H(k)$ that anticommutes with a unitary matrix $U_S$. This includes, in particular, BdG Hamiltonians in symmetry class AIII, DIII, and CI, where chiral symmetry is realized as a combination of time-reversal and particle-hole symmetry. The presence of chiral symmetry implies that $H(k)$ can be brought into block off-diagonal form

$$\tilde{H}(k) = V H(k) V^\dagger = \begin{pmatrix} 0 & D(k) \\ D^\dagger(k) & 0 \end{pmatrix},$$

(A.5)

where $V$ is a unitary transformation that brings $U_S$ into diagonal form. In order to derive the topological invariants, it is convenient to adiabatically deform $\tilde{H}(k)$ into a flat-band Hamiltonian $Q(k)$ with eigenvalues $\pm 1$. This adiabatic transformation does not alter the topological characteristics of $\tilde{H}(k)$. The flat-band Hamiltonian $Q(k)$ can be defined in terms of the spectral projector $P(k)$

$$Q(k) = \mathbb{I}_{4N} - 2P(k) = \mathbb{I}_{4N} - 2 \sum_{a=1}^{2N} \begin{pmatrix} \chi_a^-(k) \\ \eta_a^-(k) \end{pmatrix} \begin{pmatrix} [\chi_a^-(k)]^\dagger \\ [\eta_a^-(k)]^\dagger \end{pmatrix},$$

(A.6)

where $\begin{pmatrix} \chi_a^-(k) & \eta_a^-(k) \end{pmatrix}^T$ are the negative-energy eigenfunctions of $\tilde{H}(k)$, which are obtained from the eigenequation

$$\begin{pmatrix} 0 & D(k) \\ D^\dagger(k) & 0 \end{pmatrix} \begin{pmatrix} \chi_a^+(k) \\ \eta_a^+(k) \end{pmatrix} = \pm \lambda_a(k) \begin{pmatrix} \chi_a^-(k) \\ \eta_a^-(k) \end{pmatrix}. $$

(A.7)

Here, $a = 1, \ldots, 2N$ denotes the combined band and spin index. In Eq. (A.6), it is implicitly assumed that for the considered $k$ values there is a spectral gap around zero energy with $|\lambda_a(k)| > 0$, for all $a$. By multiplying Eq. (A.7) from the left by $\tilde{H}(k)$ one can show that the eigenfunctions of $\tilde{H}(k)$ can be expressed in terms of the eigenvectors $u_a(k)$ and $v_a(k)$ of $D(k)D^\dagger(k)$ and $D^\dagger(k)D(k)$, respectively,

$$D(k)D^\dagger(k)u_a(k) = \lambda_a^2(k)u_a(k), \quad D^\dagger(k)D(k)v_a(k) = \lambda_a^2(k)v_a(k),$$

(A.8)

where $u_a(k)$ and $v_a(k)$ are taken to be normalized to one, i.e., $u_a^\dagger(k)u_a(k) = v_a^\dagger(k)v_a(k) = 1$, for all $a$. That is, we have

$$\begin{pmatrix} \chi_a^\pm(k) \\ \eta_a^\pm(k) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_a(k) \\ \pm v_a(k) \end{pmatrix},$$

(A.9)
We observe that the eigenvectors of $D^\dagger(k)D(k)$ follow from $u_a(k)$ via

$$v_a(k) = N_a(k)D^\dagger(k)u_a(k),$$  \hfill (A.10)

with the normalization factor $N_a(k) = 1/\lambda_a(k)$. Combining Eqs. (A.6), (A.9), and (A.10) yields

$$Q(k) = 2N \sum_{a=1}^{2N} \begin{pmatrix} 0 & u_a(k)u_a^\dagger(k) \frac{D(k)}{\lambda_a(k)} \\ \frac{D^\dagger(k)}{\lambda_a(k)}u_a(k)u_a^\dagger(k) & 0 \end{pmatrix}. \hfill (A.11)$$

In other words, the off diagonal-block of $Q(k)$ is obtained as

$$q(k) = \sum_{a=1}^{2N} u_a(k)u_a^\dagger(k) \frac{D(k)}{\lambda_a(k)} = \begin{pmatrix} 0 & q(k) \\ q^\dagger(k) & 0 \end{pmatrix}. \hfill (A.12)$$

As shown below, both $\mathbb{Z}$ and $\mathbb{Z}_2$ topological invariants can be conveniently expressed in terms of the unitary matrix $q(k)$.

**$\mathbb{Z}$ topological invariant (winding number)**

Topologically stable Fermi surfaces (or nodal lines) in symmetry class AIII exist for even codimension $q = d_k + 1 = 2n + 2$ (see Table. 5.3). The stability of these nodal lines is guaranteed by the conservation of an integer-valued topological number, namely the winding number $\nu_{d_k=2n+1}[q]$ of $q(k)$

$$\nu_{2n+1}[q] = C_n \int_{S^{2n+1}} d^{2n+1}k \epsilon^{\mu_1\mu_2\cdots\mu_{2n+1}} \text{Tr} \left[ q^{-1}\partial_{\mu_1} q \cdot q^{-1}\partial_{\mu_2} q \cdots q^{-1}\partial_{\mu_{2n+1}} q \right], \hfill (A.13)$$

with $\epsilon^{\mu_1\mu_2\cdots\mu_{2n+1}}$ the totally antisymmetric tensor and

$$C_n = \frac{(-1)^n n!}{(2n + 1)!} \left( \frac{i}{2\pi} \right)^{n+1}. \hfill (A.14)$$

Here, $S^{2n+1}$ denotes a hypersphere in momentum space surrounding the Fermi surface (nodal line). The winding number $\nu_{2n+1}$ characterizes the topology of the occupied wavefunctions of $\mathcal{H}(k)$ restricted to $S^{2n+1}$, i.e., it describes the topology of $q(k)$ on $S^{2n+1}$. In other words, $\nu_{2n+1}[q]$ represents the homotopy number of the map $S^{2n+1} \mapsto$
\( q(k) \in U(2N) \). For \( d_k = 1 \) (i.e., \( n = 0 \)), Eq. (A.13) simplifies to

\[
\nu_1[q] = \frac{i}{2\pi} \int_{S^1} dk \text{Tr} \left[ q^{-1} \partial_k q \right] = -\frac{1}{2\pi} \text{Im} \int_{S^1} dk \text{Tr} \left[ \partial_k \ln D(k) \right],
\]

which describes the topological stability of Fermi surfaces (nodal lines) of codimension \( q = 2 \). In particular, \( \nu_1[q] \) defines the topological charge of stable nodal lines in three-dimensional time-reversal invariant superconductors [38–40] (see Secs. 3.2 and 3.3).

**Z\(_2\) topological invariant**

For time-reversal invariant superconductors in class DIII we can define, besides the winding number (A.13), also \( Z_2 \) topological numbers, provided the consider hypersphere \( S^{d_k} \) surrounding the nodal line/point is left invariant under the transformations \( k \rightarrow -k \) (see Table 5.3). In the following, we derive these \( Z_2 \) numbers for the cases \( d_k = 1 \) and \( d_k = 2 \), and assume that the centrosymmetric hyperspheres \( S^{d_k=1} \) and \( S^{d_k=2} \) contain two and four time-reversal invariant points \( K \), respectively. With these assumptions, the \( Z_2 \) topological numbers \( W_{d_k}[q] \) can be defined in terms of the Pfaffian Pf of the skewing matrix \( w_{ab}(k) \), i.e. [6,198–202],

\[
W_{d_k}[q] = \prod_{K} \frac{\text{Pf}[w(K)]}{\sqrt{\det[w(K)]}}, \quad \text{with} \quad d_k = 1, 2,
\]

where the product is over the two (four) time-reversal invariant momenta \( K \) in \( S^{d_k=1} \) (\( S^{d_k=2} \)) and

\[
w_{ab}(k) = (u^+_a(-k) | T u^+_b(k)),
\]

with \( a, b = 1, \ldots, 2N \). Here, \( u^+_a(k) \) denotes the \( a \)-th eigenvector of \( Q(k) \) with eigenvalue \( \pm 1 \), \( T = K i \sigma_2 \otimes \mathcal{K}_2N \) is the time-reversal symmetry operator, and \( K \) represents the complex conjugation operator. \( W_{d_k}[q] = +1(-1) \) indicates a topologically trivial (nontrivial) character of the enclosed Fermi surface / nodal line. Due to the block off-diagonal structure of the flat-band Hamiltonian (A.11), a set of eigenvectors of \( Q(k) \), with \( k \in S^{d_k} \), can be constructed as

\[
|u^\pm_a(k)\rangle_N = \frac{1}{\sqrt{2}} \begin{pmatrix} n_a \\ \pm q^\dagger(k)n_a \end{pmatrix},
\]

\footnote{The Pfaffian is an analog of the determinant. It is defined for \( 2n \times 2n \) antisymmetric matrices \( A \) and can be expressed in terms of a sum over all elements of the permutation group \( S_{2n} \),

\[
Pf(A) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) \prod_{i=1}^n A_{\sigma(2i-1), \sigma(2i)}.\]}

The Pfaffian is an analog of the determinant. It is defined for \( 2n \times 2n \) antisymmetric matrices \( A \) and can be expressed in terms of a sum over all elements of the permutation group \( S_{2n} \),

\[
Pf(A) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) \prod_{i=1}^n A_{\sigma(2i-1), \sigma(2i)}.\]
or, alternatively, as

\[ |u_{a}^{\pm}(k)\rangle_{S} = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \pm q(k)n_{a} \\ n_{a} \end{array} \right), \]  

(A.19)

where \( n_{a} \) are \( 2N \) momentum-independent orthonormal vectors. For simplicity we choose \( (n_{a})_{b} = \delta_{ab} \). Observe that both \( |u_{a}^{\pm}(k)\rangle_{N} \) and \( |u_{a}^{\pm}(k)\rangle_{S} \), with \( k \in S^{d_{k}} \), are well-defined globally over the entire hypersphere \( S^{d_{k}} \). In the following we work with the basis \( |u_{a}^{\pm}(k)\rangle_{N} \). Eq. (A.17) together with Eq. (A.18) gives

\[ w_{ab}(k) = \frac{1}{2} \left( n_{a}^{T} q(k) n_{b} - n_{b}^{T} q(-k) n_{a} \right) = q^{T}_{ab}(k). \]  

(A.20)

In going from the second to the third line in Eq. (A.20), we used the fact that due to time-reversal symmetry \( q(-k) = -q^{T}(k) \). Thus, the \( \mathbb{Z}_{2} \) topological number \( W_{d_{k}}[q] \) for \( d_{k} = 1 \) and \( d_{k} = 2 \) is

\[ W_{d_{k}}[q] = \prod_{K} Pf \left[ q^{T}(K) \right] \]  

(A.21)

with \( K \) the two (four) time-reversal invariant momenta of \( S^{d_{k}=1} \) (\( S^{d_{k}=2} \)).
Appendix B

B.1 Continuum BdG equations

The continuum BdG equation can be expressed as

\[ H \psi = \begin{pmatrix} h & \Delta \\ \Delta^\dagger & -h^* \end{pmatrix} \psi = E \psi, \] (B.1)

where \( h = ( -\frac{\nabla^2}{2m} - \mu ) 1_{2\times2} + \alpha l(k) \cdot \sigma \), with \( m \) the effective mass, \( \mu \) the chemical potential, and \( \alpha l(k) \cdot \sigma \) the Rashba-type SOC with strength \( \alpha \). The pairing term has the form \( \Delta = (\Delta_s + \frac{1}{2} \nabla \cdot D + D \cdot \nabla)(i\sigma_2) \), where \( \Delta_s \) is the singlet pairing amplitude and \( D = -i\nabla_k (\Delta_p l(k) \cdot \sigma) \) presents the triplet pairing. Here, \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \) is the vector of Pauli matrices. Without loss of generality, we consider the spin-orbit coupling vector \( l(k) = (a_1 k_y + a_4 k_y + a_4 k_x, a_3 k_z) \). A vortex line along the \( z \) direction can be introduced by adding a phase on both singlet and triplet pairing amplitudes, \( \Delta_s \rightarrow e^{i\theta} \Delta_s \) and \( \Delta_t \rightarrow e^{i\theta} \Delta_t \). In the cylindrical coordinate, the normal-state Hamiltonian and the pairing term are

\[
\begin{align*}
\Delta_s & = e^{i\theta} \Delta_s \\
\Delta_t & = -i \Delta_t
\end{align*}
\]

\[
\begin{pmatrix}
\Delta_s e^{i\theta} (i\sigma_2) \\
-i \Delta_t
\end{pmatrix}
\begin{pmatrix}
a_3(-i\partial_z) & -ia_1 e^{-i\theta} (\partial_r - \frac{1}{r} \partial_{\theta}) - ia_4 e^{i\theta} (-i\partial_r + \frac{1}{r} \partial_{\theta}) \\
-ia_1 e^{i\theta} (\partial_r + \frac{1}{r} \partial_{\theta}) - ia_4 e^{-i\theta} (i\partial_r + \frac{1}{r} \partial_{\theta}) & a_3(i\partial_z)
\end{pmatrix},
\]

\[
\begin{pmatrix}
ah \left( -\frac{1}{2m} (\partial^2_r + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial^2_{\theta} + \partial^2_z) - \mu \right) 1_{2\times2} \\
+ \alpha
\begin{pmatrix}
\begin{pmatrix} a_3(-i\partial_z) & -ia_1 e^{-i\theta} (\partial_r - \frac{1}{r} \partial_{\theta}) - ia_4 e^{i\theta} (-i\partial_r + \frac{1}{r} \partial_{\theta}) \\
-ia_1 e^{i\theta} (\partial_r + \frac{1}{r} \partial_{\theta}) - ia_4 e^{-i\theta} (i\partial_r + \frac{1}{r} \partial_{\theta}) & a_3(i\partial_z)
\end{pmatrix}
\end{pmatrix}
\end{pmatrix},
\]

(151)
A general solution of this continuum BdG equation is \( \psi(r, \theta, z) = e^{ikz}[\tilde{u}_\uparrow(r)e^{i\mu_1\theta}, \tilde{u}_\downarrow(r)e^{i\mu_2\theta}, \tilde{v}_\uparrow(r)e^{i\mu_3\theta}, \tilde{v}_\downarrow(r)e^{i\mu_4\theta}]^T \).

The radial part of a localized solution must be of the form \( f(r) \sim e^{-\kappa r} \) with Re[\( \kappa \)] > 0. In the asymptotic limit \( (1/r \rightarrow 0) \), we can neglect all \( \frac{1}{r^4} \) and \( \frac{1}{r^7} \) terms. We find for \( (m_1, m_2, n_1, n_2) = (0, 1, 0, -1) \) and \( a_4 = 0 \), that the continuum BdG equation has a localized zero-energy solution for (i) \( k_z = 0 \) or (ii) \( a_3 = 0 \), that satisfies

\[
\begin{pmatrix}
-\frac{1}{2m}\kappa^2 - \mu & i\alpha a_1\kappa e^{-i\theta} & -i\Delta_1a_1\kappa & \Delta_2 e^{i\theta} \\
 i\alpha a_1\kappa e^{i\theta} & -\frac{1}{2m}\kappa^2 - \mu & -\Delta_2 e^{i\theta} & i\Delta_1a_1\kappa e^{2i\theta} \\
 i\Delta_1a_1\kappa & -\Delta_2 e^{-i\theta} & \frac{1}{2m}\kappa^2 + \mu & -i\alpha a_1\kappa e^{i\theta} \\
 \Delta_2 e^{-i\theta} & -i\Delta_1a_1\kappa e^{-2i\theta} & -i\alpha a_1\kappa e^{-i\theta} & \frac{1}{2m}\kappa^2 + \mu
\end{pmatrix}
\begin{pmatrix}
\tilde{u}_\uparrow(r) \\
\tilde{u}_\downarrow(r) \\
\tilde{v}_\uparrow(r) \\
\tilde{v}_\downarrow(r)
\end{pmatrix}
= 0. \quad (B.3)
\]

Note that this situation corresponds to a zero-energy bound-state solution at \( k_z = 0 \) for the \( D_4 \) point-group NCS. In addition, the decay length \( \kappa \) is determined by solving the roots of the following determinant

\[
\text{Det}
\begin{pmatrix}
-\frac{1}{2m}\kappa^2 - \mu & i\alpha a_1\kappa & -i\Delta_1a_1\kappa & \Delta_2 \\
i\alpha a_1\kappa & -\frac{1}{2m}\kappa^2 - \mu & -\Delta_2 & i\Delta_1a_1\kappa \\
i\Delta_1a_1\kappa & -\Delta_2 & \frac{1}{2m}\kappa^2 + \mu & -i\alpha a_1\kappa \\
\Delta_2 & -i\Delta_1a_1\kappa & -i\alpha a_1\kappa & \frac{1}{2m}\kappa^2 + \mu
\end{pmatrix}
= 0. \quad (B.4)
\]

There are only two decaying solutions (Re[\( \kappa \)] > 0)

\[
\kappa_{\pm} = \sqrt{-2a_1^2m^2(\alpha^2 + \Delta_2^2) - 2m\mu \pm 2\sqrt{[a_1^2m^2(\alpha^2 + \Delta_2^2) + m\mu]^2 - m^2(\Delta_2^2 + \mu^2)}}, \quad (B.5)
\]

with the condition

\[
-a_1^2m^2(\alpha^2 + \Delta_2^2) - m\mu - \text{Re} \left[ \sqrt{[a_1^2m^2(\alpha^2 + \Delta_2^2) + m\mu]^2 - m^2(\Delta_2^2 + \mu^2)} \right] > 0. \quad (B.6)
\]

### B.2 Higher-order SOC in NCSs with \( C_{4v} \) point-group symmetry

For the \( C_{4v} \) NCS with \( l(k) \) given by Eq. (4.3b) (i.e., only the lowest order SOC term) one finds that the BdG Hamiltonian \( H(k) \) is an even function of \( k_z \). Hence, an effective two-dimensional layer with fixed \( k_z \) satisfies time-reversal and particle-hole symmetries, \( U_T^{-1}H(k_x, k_y)U_T = H^*(-k_x, -k_y) \) and \( U_P^{-1}H(k_x, k_y)U_P = -H^*(-k_x, -k_y) \). It turns out that each layer with fixed \( k_z \) belongs to class DIII and the two-dimensional \( \mathbb{Z}_2 \) topological invariant \( (4.10) \) can be computed. For \( k_z \) within the two nodal rings, we find that the \( \mathbb{Z}_2 \) number takes on a nontrivial value, which
Figure B.1: (Color online). Energy spectrum as a function of \( k_z \) of a \( C_{4v} \) NCS with \( (a_1, a_2) = (1.0, 2.0), \mu = -2.5, \) and \( \Delta_s = 0.5. \) (a) Without vortices and OBC along the \( x \) axis but PBCs in the other two directions. (b) With a pair of vortex-antivortex lines oriented along the \( z \) axis and PBCs in all three directions.

leads to the appearance of helical arc surface states.

It is interesting to ask whether this reasoning remains valid upon inclusion of higher-order terms in the spin-orbit interaction. Up to second order the SOC vector \( l(k) \) for the \( C_{4v} \) point-group is given by

\[
l(k) = a_1 [\sin k_y \hat{e}_1 - \sin k_x \hat{e}_2] + a_2 \sin k_x \sin k_y \sin k_z (\cos k_x - \cos k_y) \hat{e}_3.
\]

We observe that the second-order term is an odd function of \( k_z \), and hence two-dimensional layers with fixed \( k_z \) are no longer symmetric under TRS and PHS. Our numerics shows that upon inclusion of the second-order term with \( a_2 \neq 0 \), the flat-band vortex-bound states become dispersive [Fig. B.1(b)]. However, the arc surface states remain unaffected [Fig. B.1(a)]. It turns out that the arc surface states on the (010) and (100) faces are protected by a reflection symmetry which leaves the surface plane invariant. The Hamiltonian in a (010) slab geometry is invariant under the following reflection symmetry:

\[
U_{R_x}^\dagger \tilde{\mathcal{H}}(y, y'; k_x, k_z) U_{R_x} = \tilde{\mathcal{H}}(y, y'; -k_x, k_z), \tag{B.7}
\]

with \( U_{R_x} = \delta_{y,y} \otimes [\sigma_3 \otimes \sigma_1] \), where \( \delta_{y,y} \) acts on the real-space basis and \( \sigma_3 \otimes \sigma_1 \) acts on the momentum-space Nambu basis. The Hamiltonian in a (100) geometry, on the other hand, is invariant under the following mirror symmetry:

\[
U_{R_y}^\dagger \tilde{\mathcal{H}}(x, x'; k_y, k_z) U_{R_y} = \tilde{\mathcal{H}}(x, x'; -k_y, k_z), \tag{B.8}
\]

with \( U_{R_y} = \delta_{x,x} \otimes [I_{2 \times 2} \otimes \sigma_2] \), where \( \delta_{x,x} \) acts on the real-space basis and \( I_{2 \times 2} \otimes \sigma_2 \) acts on the momentum-space Nambu basis. Here, \( \tilde{\mathcal{H}}(y, y'; k_x, k_z) \) and \( \tilde{\mathcal{H}}(x, x'; k_y, k_z) \) represent the tight-binding Hamiltonians of the \( C_{4v} \) NCS.
in a (010) and (100) slab geometry, respectively. Note that the arc surface states on the (010) face [(100) face] are
left invariant by the reflection symmetry $R_x$ [$R_y$] and that both reflection operators $U_{R_x}$ and $U_{R_y}$ have eigenvalues
$+1$ and $-1$. Since the reflection operator $U_{R_x}$ [$U_{R_y}$] commutes with $\tilde{\mathcal{H}}(y, y'; k_x = 0, k_z)$ [$\tilde{\mathcal{H}}(x, x'; k_y = 0, k_z)$],
the eigenfunctions of $\tilde{\mathcal{H}}(y, y'; k_x = 0, k_z)$ [$\tilde{\mathcal{H}}(x, x'; k_y = 0, k_z)$] are simultaneous eigenstates of $U_{R_x}$ [$U_{R_y}$] with
eigenvalues $+1$ or $-1$. We have checked that the two helical zero-energy surface states belong to different eigenspaces
of $U_{R_x}$ [$U_{R_y}$]. Thus these zero-energy states cannot hybridize and are protected by these reflection symmetries.
Appendix C

C.1 Dimension-raising and dimension-lowering maps

We will present isomorphic maps from Hamiltonians on a $d$-dimensional sphere to Hamiltonians on a $(d + 1)$-dimensional sphere following Refs. [55, 111].

C.1.1 Hamiltonian mapping

Let us consider a Hamiltonian $H(r, k)$ on a $(d_1 + d_2)$-dimensional sphere $S^{d_1 + d_2}$. The symmetry removing (adding) mappings that sent a Hamiltonian $H_c(r, k)$ ($H_{nc}(r, k)$) with (without) chiral symmetry to a Hamiltonian without (with) chiral symmetry in the following

$$H_{nc}(r, k, \theta) = \sin \theta H_c(r, k) + \cos \theta S, \quad \theta \in [0, \pi], \quad \text{(C.1)}$$

$$H_c(r, k, \theta) = \sin \theta H_{nc}(r, k) \otimes \tau_z + \cos \theta I \otimes \tau_\alpha, \quad \theta \in [0, \pi], \quad \text{(C.2)}$$

where $H_c(H_{nc})$ denotes the presence (absence) of chiral symmetry in the Hamiltonian, $S$ is the chiral symmetry operator for the original Hamiltonian $H_c(\kappa)$, and $\alpha = x$ (or $y$) depends on the original Hamiltonian $H_{nc}(\kappa)$ with TRS (or PHS). For the complex classes, the chiral symmetry for the mapped Hamiltonian is $S = I \otimes \tau_z \tau_\alpha$.

The mapped Hamiltonian is independent at $\theta = 0$ and $\theta = \pi$. At these two points, we can consider the base space $S^{d_1 + d_2}$ to be contracted to a point. Thus the mapped Hamiltonian is defined on the $S^{d_1 + d_2 + 1}$.

C.1.2 Invertibility

In order to prove the dimension-raising mappings are isomorphic, we need to show that an inverse exists. The inversion mappings are constructed from Morse theory[203]. Let us consider a Hamiltonian $H(r, k, \theta)$ on a $(d_1 + d_2 + 1)$-dimensional sphere, which is no $(k, r)$ dependent at $\theta = 0$ and $\theta = \pi$. This condition gives two boundary
conditions

\[ \mathcal{H}(r, k, \theta = 0) = \text{const.}, \quad \mathcal{H}(r, k, \theta = \pi) = \text{const}'. \]

(C.3)

To show this Hamiltonian can be continuously deformed to Eqs. (C.1) and (C.2), we introduce an artificial action

\[ S[\mathcal{H}(r, k, \theta)] = \int d\theta d^{d_{1}}r d^{d_{2}}k \text{Tr}(\partial_{\theta} \mathcal{H} \partial_{\theta} \mathcal{H}) \]

(C.4)

In addition, we also flatten this Hamiltonian under continuous deformation \( \mathcal{H}(r, k, \theta)^{2} = 1 \). Thus the saddle point equation gives

\[ \partial_{\theta}^{2} \mathcal{H} + \mathcal{H} = 0. \]

(C.5)

Combining this saddle point equation, the boundary conditions, and flatness condition, the Hamiltonian has the form

\[ \mathcal{H}(r, k, \theta) = \sin \theta \mathcal{H}_{1}(r, k) + \cos \theta \mathcal{H}_{0}, \]

(C.6)

with

\[ \mathcal{H}_{1}(r, k)^{2} = \mathcal{H}_{0}^{2} = 1, \quad \{\mathcal{H}_{1}(r, k), \mathcal{H}_{0}\} = 0. \]

(C.7)

By fixing \( \theta = \pi/2 \), we have a dimensional reduction \( \mathcal{H}(r, k, \theta) \rightarrow \mathcal{H}_{1}(r, k) \).

If \( \mathcal{H}(r, k, \theta) \) is non-chiral, then \( \mathcal{H}_{c}(r, k) = \mathcal{H}_{1}(r, k) \) is chiral symmetric with \( S = \mathcal{H}_{0} \). Hence Eq. (C.1) are invertible when \( s \) is odd. On the other hand, if \( \mathcal{H}(r, k, \theta) \) is chiral, there exists a chiral symmetry operator \( S \) that anticommutes with both \( \mathcal{H}_{1}(r, k) \) and \( \mathcal{H}_{0} \). By defining \( S = \mathbb{1} \otimes \tau_{z} \), \( \mathcal{H}_{0} = \mathbb{1} \otimes \tau_{y} \), and \( \mathcal{H}_{1}(r, k) = h(r, k) \otimes \tau_{z} \), the Hamiltonian is

\[ \mathcal{H}(r, k, \theta) = \sin \theta h(r, k) \otimes \tau_{z} + \cos \theta \mathbb{1} \otimes \tau_{y}, \]

(C.8)

which takes the form of Eq. (C.2) with \( \mathcal{H}_{nc}(r, k) = h(r, k) \). Since \( h(r, k) \) is non-chiral, we show that Eq. (C.2) are invertible when \( s \) is even.
References


