Majorana Quasiparticles in Topological Material Interfaces

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MAJORANA QUASIPARTICLES IN TOPOLOGICAL MATERIAL INTERFACES

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Abstract

In this dissertation we analyze how Majorana quasiparticles found on material interfaces of both topological insulators (TIs) and topological superconductors (TSCs) are affected by imperfections within their local environment. While these quasiparticles are predicted to be critical for the construction of quantum computers, they are typically modeled only under pristine conditions. Thus, although quantum computers may require the spatial manipulation of Majorana quasiparticles, these topological material interfaces are commonly studied in static contexts and their response to manipulation remains an open question. We first demonstrate that interface potentials on the topological insulator Bi$_2$Se$_3$ can enable the emergence of Majorana bound states. Specifically, we study how non-helical spin-textures at the boundaries between TIs and SCs affect the proximity-induced superconductivity of the TI-interface state. We furthermore show that the Andreev conductance of lateral heterostructures joining TI-vacuum and TI-SC interfaces yields experimental signatures of the reduced symmetries of the interface. Next, we study the in-gap states that appear at the boundaries of both one-dimensional and two-dimensional TSCs. While massless Majorana quasiparticles are guaranteed to arise by the bulk-boundary correspondence, we find that they could be accompanied by massive Volkov-Pankratov (VP) states which are present only when the interface is sufficiently smooth. We calculate the spin-resolved local density of states of the VP states about the band inversion generated by a magnetic domain wall and find that they are oppositely spin polarized on either side of the topological phase boundary. Finally, we study how topological phase transitions in two-dimensional nanoflakes can be driven not only through magnetic domain walls but additionally through local changes in the system’s chemical potential. We calculate the spatial extent of the one-dimensional Majorana modes circulating the boundary of the nanoflake and numerically determine their energy eigenvalues.
Chapter 1. Introduction

As the next generation of technology draws near, devices based on quantum phenomena have been promised to provide radical new developments in the construction of computers, detectors, and methods of communication [1]. Currently envisioned devices such as the quantum computer would give rise to advanced cryptography for more secure communication, and computational capabilities significantly larger than those possible in classical computing and at far greater speeds. Only recently have these next-generation technologies been incorporated into devices which have demonstrated performance rivaling those of their conventional counterparts [2].

Modern proposals for the fabrication of these devices rely on the use of “topological” materials whose surfaces behave differently than their bulk. Some examples of these include Bi$_2$Se$_3$ and HgTe quantum wells, both of which are topological insulators that conduct electricity on their boundaries [3, 4]. Quantum computers rely on the use of quantum two-level systems known as qubits. These qubits can be sensitive to perturbations and prone to decoherence which impedes their ability to encode information. Topological qubits, or qubits formed on the interfaces of topological materials, are predicted to be immune to local sources of disturbance and are among the most stable of possible candidates [5, 6]. Realizing these devices requires detailed understanding along with precise control of quantum material interfaces. However, the existing theoretical literature has modeled these materials as if they were isolated in space, and do not address how junctions between these materials can alter their behavior. Furthermore, finding nondestructive methods to manipulate topological qubits remains an open question.

The consequences of imperfections at junctions between topological materials can be critical, as nontrivial interface effects can both suppress and assist in the appearance of these topological qubits [7, 8]. In this dissertation we analyze how non-ideal interfaces affect the behavior of topological materials for their use in next-generation technologies.
1.1. Majorana Quasiparticles as a Platform for Topological Quantum Computations

In 1937 the Italian physicist Ettore Majorana modified the relativistic Dirac equation in an attempt to model electrically neutral neutrinos [9]. He demonstrated that if the wave functions in the Dirac equation were purely real-valued, then the neutrino may behave as its own antiparticle. While the observation of neutrinoless double beta decay would confirm this hypothesis, it has yet to be experimentally confirmed. To date, no fundamental particles have been found which behave as Majorana fermions.

Condensed matter systems offer a novel platform for the observation of Majorana fermions; here they do not arise as fundamental particles, but instead as many-body quasiparticle excitations. Superconductors (SCs), for instance, naturally offer an environment where the quasiparticle excitations are equal superpositions of electrons and holes known as Cooper pairs [10]. Under the presence of strong spin-orbit coupling (SOC) and an external magnetization, the SC begins to host zero-energy vortex excitations which behave as their own antiparticles and fulfill Majorana’s condition [11]. If the SC is two-dimensional then these Majorana quasiparticles exhibit another special property: they behave as objects known as non-abelian anyons [6]. This means that the ground state of several Majorana quasiparticles is degenerate, and the system enters into distinct new states as the quasiparticles are spatially moved around one-another. This process is known as “braiding” and is how Majorana quasiparticles can encode quantum information while always remaining at zero energy, and thereby allowing the system to be insensitive to perturbations.

1.2. Topological Insulators and Topological Superconductors

To realize Majorana quasiparticles we must search for a low-dimensional system with both superconductivity and strong SOC. It turns out that material interfaces between topological materials and trivial (i.e., non-topological) SCs contain both of these necessary ingredients.

Topological insulators (TIs) are a class of materials that behave as insulators within their bulk, but admit topologically-protected conducting metallic edge states on their sur-
faces. Bi$_2$Se$_3$ and HgTe quantum wells are three-dimensional and two-dimensional TIs respectively [3, 4]. While traditionally the phase of a material is defined by the presence or absence of certain symmetries, these materials respect the same global symmetry as trivial insulators, namely time-reversal symmetry. The different phases of topological and trivial insulators are incapable of being defined through the formalism of spontaneous symmetry breaking, and instead must be defined through their topology. Even though the definition of a material’s topology depends on the specific properties of its Hamiltonian, the statement of bulk-boundary correspondence shows that topologically nontrivial insulators can be identified through the existence of gapless states in their band structure localized on their boundaries. This can be qualitatively understood by noting that the vacuum may be treated as a material in a topologically trivial phase, and therefore the surface of the TI constitutes a region of a topological phase transition.

These localized states at the TI’s boundary are not typical metallic states. Due to the linearity of their band structure, they behave as massless relativistic Dirac particles [4]. In addition time-reversal symmetry forces these states to have a very specific spin structure. The surface states are helical eigenstates with their spin locked perpendicular to the direction of their momentum, and confined within the plane of the interface. This spin-momentum locking can be modeled as an infinite strength SOC [12].

In 2008, Liang Fu and Charles L. Kane predicted that placing a TI in proximity to both a SC and a ferromagnetic insulator can lead to the appearance of Majorana fermions [5]. The topological surface states become superconducting due to the proximity effect, and therefore lead to electrically neutral particle-hole excitations with strong SOC. The ferromagnetic insulator gives rise to a magnetization leading to the appearance of Majorana quasiparticles.

Despite many observations which are consistent with Majorana quasiparticle behavior, there has been no smoking-gun experimental evidence of their existence to date. One obstacle arises from magnetic impurities on the TI surface which can lead to the formation of additional states with extremely low nonzero energies. Determining if an excitation is truly
Figure 1.1. (a) A Topological Insulator (TI) is shown with its surface state. (b) By placing the TI next to a superconductor (SC) in a magnetic field $\mathbf{B}$, the interface electrons form vortices that can host topological qubits.

zero-energy Majorana state compared to a low-lying impurity state requires an energy resolution which is beyond the scope of modern-day experimental techniques. Understanding the effects of material imperfections at the TI surface is therefore vital for the experimental confirmation of Majorana quasiparticles.

Another class of materials with similar properties are topological superconductors (TSCs). SCs can be modeled similarly to insulators as they both have energy gaps in their band structure. Like TIs, TSCs exhibit zero-energy states at their boundaries. Unlike TIs, these zero-energy edge states are intrinsically Majorana quasiparticles. While there are many known and affordably available TIs, there are currently no known examples of TSCs. Despite this, low-dimensional SCs with strong SOC, such as Pb monolayers, can experience topological phase transitions under the presence of spatially varying magnetizations [8, 11, 13, 14].

1.3. Consequences of Material Interfaces

In both of the examples of TIs and TSCs, the Majorana quasiparticles exist as localized objects at certain edges and boundaries. As previously discussed, these quasiparticles are non-abelian anyons that need to be spatially moved around one another in order to encode
quantum information. While the above proposals are theoretically well-established, there are currently few proposals which address how these Majorana modes can be spatially controlled. Here the consequences of imperfections again become critical, as attempts to move these quasiparticles in space can affect their desired behavior.

To answer these currently open questions, this dissertation is structured in the following way: In Chapter 2, we study crystalline heterostructures which comprise TIs in contact with SCs, and demonstrate that interface potentials between these two materials can enable the emergence of Majorana bound states. For parent s-wave SCs, the electrons of the TI’s interface state feel superconductivity due to the proximity effect. However, for other species of parent SCs such as chiral $p_x + ip_y$ SCs, superconductivity is not projected onto the TI-SC interface and thus Majorana bound states are unable to form. We demonstrate that interface potentials, such as those which come from shear stresses and strain between the materials, enable the emergence of the superconducting proximity effect and thus the presence of Majorana bound states. Focusing on chiral $p_x + ip_y$ SCs, we then study the experimental consequences of these effects by analyzing the Andreev conductance spectra of lateral heterojunctions, which may be created by covering only half of a TI surface with a SC. The incoming electronic TI surface states enter into the superconducting TI-SC region, and the total conductance is therefore controlled by the shear- and strain-induced interface potentials of the TI-SC boundary. In Chapter 3, we derive the theoretical framework necessary to relate the wave functions of the TI-vacuum and TI-SC regions using the hermiticity of the total system Hamiltonian, and study the consequences interface potentials have on the conductance spectra of lateral heterojunctions with both parent s-wave and various spin-triplet SCs.

In Chapter 4 we study the consequences of smoothly-varying magnetic domain walls in both one-dimensional and two-dimensional SCs with large Rashba SOC. Recent experimental work has shown that two-dimensional Pb monolayers may host one-dimensional chiral Majorana bound states [13, 14]. These Pb monolayers exhibit strong Rashba SOC. When
combined with a magnetic Zeeman exchanged field arising from magnetic Co islands deposited in the Si substrate supporting the Pb, the superconducting system has the sufficient ingredients necessary to exhibit Majorana bound states on the boundaries of the Co islands. However, while the language of topology only predicts the presence of these zero-energy Majorana states, the experimental data also revealed additional states at higher and lower energies, which split away from the Co island boundaries. We derive a theoretical model that shows these additional states, known as Volkov-Pankratov (VP) states, emerge as a consequence of a smoothly-varying domain wall, as opposed to a discrete change between magnetic and non-magnetic regions. We calculate the spin-resolved local density of states of the system, and show that the VP states are strongly spin-polarized, with opposite spin polarizations on opposite sides of the magnetic domain wall. We also calculate the effect of in-plane electric fields, and show that they can introduce additional VP states below the superconducting energy gap of the system.

In Chapter 5 we continue our analysis of two-dimensional SCs and chiral Majorana bound states. However, we show that instead of using magnetic domain walls, Majorana bound states can also emerge in systems held at a constant Magnetic Zeeman energy as long as there is a spatially varying chemical potential [11]. Here we explicitly study the case in which a circular nanoflake is deposited on a SC, creating a localized region with a modified chemical potential and resulting in a one-dimensional chiral Majorana bound state at its circumference. We calculate the spatial extent of these radially symmetric states in terms of the system parameters, and numerically determine their energy eigenvalues.

In Chapter 6, we summarize the results of our work and discuss how each of these directions help inform us on the potential utilization of Majorana fermions in next-generation devices.
Chapter 2. Proximity-Induced Superconductivity at Nonhelical Topological Insulator Interfaces

2.1. Introduction

Topological insulators (TIs) are a class of materials which belong to a distinct phase separate from their trivial counterparts despite respecting the same global symmetries [15, 16]. The main signature of this phase is the presence of linearly dispersing metallic states at the boundaries of the TI. These states are robust under perturbations that preserve time reversal symmetry, and as a consequence of the bulk spin-orbit interaction their spin and momenta are locked relative to each other.

At planar TI-vacuum terminations these gapless surface states have isotropic dispersions, are perfectly helical (with their spin normal to the direction of their momentum and confined in the interface plane), and can be described by a two-dimensional massless-Dirac effective Hamiltonian. It is commonly assumed that interfaces within heterostructures of TIs and topologically trivial materials exhibit these same properties. However, effects due to lattice strain, charge redistribution, dangling bonds, and other non-magnetic interface potentials may lower the symmetry of the interface relative to the bulk. It was recently shown that metallic states at the interface reflect these reduced symmetries, so that generally their dispersion is anisotropic and the spin-momentum locking is not helical [17].

Some of the most promising potential applications of TIs rely on the proximity-induced superconductivity from a TI interface state in contact with a bulk superconductor (SC) [5]. When vortices are present or when placed alongside ferromagnetic systems, these junctions are predicted to host Majorana fermions, which are critical for fault-tolerant quantum computing [5, 18]. However, the properties of the induced superconductivity strongly depend on the spin structure of the interface state as well as the properties of the parent SC. Existing conclusions about the interface superconductivity, including the prediction that some spin-

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triplet parent SCs do not induce superconductivity in the interface state at all [19], have been reached assuming helical TI surface states.

In this chapter we analyze proximity-induced superconductivity in TI-SC heterostructures assuming the most general form of the interface state allowed by symmetry. We obtain the superconducting order parameter at the interface and demonstrate that when the parent SC is spin-singlet, the shape of the induced superconducting gap mimics that of the parent. For spin-triplet parent SCs on the other hand, distinct anisotropic phases emerge depending on the nature of the interface. Strikingly, interface potentials may enable proximity-induced superconductivity for spin-triplet SCs that do not induce superconductivity in the helical Dirac states. One such example is the chiral state suggested for Sr$_2$RuO$_4$ [20], which requires
out-of-plane spin textures in the TI interface state. In addition, we show that conductance spectroscopy of lateral heterostructures of TI-vacuum and TI-SC interfaces exhibits clear signatures of symmetry-breaking interface potentials.

2.2. Model for the Interface States

To describe TI interface states, we start from the most general time-reversal invariant Hamiltonian that is linear in momentum:

\[ H(k) = c(k) \cdot \sigma. \]  

(2.1)

Here, \( k = (k_x, k_y)^T \) is the in-plane momentum, \( \sigma = (\sigma_x, \sigma_y, \sigma_z)^T \) is a vector of Pauli matrices in spin space, and \( c(k) \) is a three-dimensional vector such that \( c_i(k) = \sum_j c_{ij} k_j \) with real coefficients \( c_{ij} \), where \( i \in \{x, y, z\} \) and \( j \in \{x, y\} \). We contrast the general Hamiltonian Eq. (2.1) with the well-known Dirac Hamiltonian describing the low-energy physics of TI surface states, \( H_D(k) = \hbar v_F (\sigma \times k)_z \), which is obtained for the choice \( c_D(k) = \hbar v_F (k_y, -k_x, 0) \) where \( v_F \) is the Fermi velocity.

Due to the mismatch of the basis functions it is generally difficult to develop reliable effective models for SC-semiconductor heterostructures [21], and especially so for topological systems [22]. While \( H_D(k) \) is often believed to hold for idealized interfaces of TIs with non-topological materials, Ref. [17] showed that non-magnetic interface potentials generally lead to an interface described by Eq. (2.1) with modified coefficients \( c_{ij} \), whose values are determined by the material-specific details in the microscopic calculations. The general form of these coefficients however can be determined by imposing spatial symmetries at the interface, and therefore we use Eq. (2.1) as a general starting point to analyze the proximity effect in TI-SC heterostructures. The description of the TI interface states via Eq. (2.1) is valid as long as the coupling between the TI and the SC is small, so that the interface states retain their topological character [22, 23].
2.3. Interface Superconductivity

Since \( c(k) = -c(-k) \), the form of the Hamiltonian in Eq. (2.1) is identical to that of antisymmetric spin-orbit coupling in non-centrosymmetric metals, whose influence on superconducting pairing has been extensively studied [24, 25]. The key difference is that the regular quadratic kinetic energy term is absent, placing us in the limit of infinitely strong spin-orbit coupling [12]. Consequently, only one of the spin-orbit split bands crosses the chemical potential, and the quasiparticles that form Cooper pairs at the TI interface are effectively spinless.

In this limit, and under the assumption of weak TI-SC coupling, the proximity-induced superconducting order in the interface layer can be adequately described by simply projecting the Cooper pair structure of the parent SC, \( \hat{\Delta} = [\psi(k) + d(k) \cdot \sigma](i\sigma_y) \) where \( \psi(k) \) and \( d(k) \) are the spin-singlet and spin-triplet parts of the pairing field respectively, onto the eigenstates of the interface Hamiltonian. Writing the electron field operators as \((a_k^\uparrow, a_k^\downarrow)\), and introducing the Nambu spinor \( \Psi = (a_k^\uparrow, a_k^\downarrow, a_{-k}^\dagger^\uparrow, a_{-k}^\dagger^\downarrow)^T \), the Bogoliubov-de Gennes (BdG) Hamiltonian becomes

\[
\mathcal{H} = \frac{1}{2} \sum_k \Psi^\dagger \begin{pmatrix} H(k) - \mu & \hat{\Delta} \\ \hat{\Delta}^\dagger & -H^T(-k) + \mu \end{pmatrix} \Psi. 
\]

(2.2)

Here \( \mu \) is the chemical potential. Transforming to the band representation, denoting the annihilation operators for the eigenstates of the conduction and the valence bands in Eq. (2.1) as \((b_{k1}, b_{k2})\) respectively, and introducing the corresponding band Nambu spinor
\[ \Phi = (b_{k1}, b_{k2}, b_{-k1}^\dagger, b_{-k2}^\dagger)^T \]

we arrive at the mean field pairing Hamiltonian for the interface,

\[
\mathcal{H} = \frac{1}{2} \sum_k \Phi^\dagger \times \begin{pmatrix}
|c| - \mu & 0 & -e^{-i\varphi_c}[\hat{c} \cdot d + \psi] & \frac{[\hat{c} \times (\hat{c} \times d)]_0 - i(\hat{c} \times d)_z}{e^{i\varphi_c} \sin \vartheta_c} \\
0 & |c| - \mu & -e^{i\varphi_c}[\hat{c} \cdot d - \psi] & \frac{[\hat{c} \times (\hat{c} \times d)]_0 + i(\hat{c} \times d)_z}{e^{i\varphi_c} \sin \vartheta_c} \\
-e^{i\varphi_c}[\hat{c} \cdot d^* + \psi^*] & -e^{-i\varphi_c}[\hat{c} \cdot d^* - \psi^*] & |c| + \mu & 0 \\
\frac{[\hat{c} \times (\hat{c} \times d^*)]_0 + i(\hat{c} \times d^*)_z}{e^{i\varphi_c} \sin \vartheta_c} & \frac{[\hat{c} \times (\hat{c} \times d^*)]_0 - i(\hat{c} \times d^*)_z}{e^{i\varphi_c} \sin \vartheta_c} & 0 & |c| + \mu
\end{pmatrix} \Phi.
\] (2.3)

Here \( \hat{c}(k) \) is the unit vector along \( c(k) \) and \( \vartheta_c(k) \), \( \varphi_c(k) \) are the polar and azimuthal angles of the vector \( c(k) \), respectively. For brevity in Eq. (2.3) we omitted the argument \( k \), but the momentum dependence is implicit in all of the functions. In principle, Eq. (2.3) contains all possible superconducting order parameters allowed in a TI-SC heterostructure, including both the intra- and inter-band pairing of the interface states. Below, we focus on the experimentally relevant situation where the chemical potential is far away from the charge neutrality point. In this case the system is in the weak-coupling limit defined by \( \mu \gg |\psi(k)|, |d(k)| \) and only a single, nondegenerate band crosses the Fermi level. The matrix elements on the antidiagonal of Eq. (2.3) correspond to interband pairing between the states of this conduction band with states that are far away from the Fermi surface, and therefore can be neglected due to the large energy mismatch. From Eq. (2.3) we can see that the order parameter for the spinless fermions in the conduction band takes the form

\[
\Delta(k) = -e^{-i\varphi_c(k)}[\hat{c}(k) \cdot d(k) + \psi(k)].
\] (2.4)

The implications of Eq. (2.4) are distinct for the cases of singlet and triplet SCs. In the singlet case, the momentum dependence of the gap magnitude \( |\Delta(k)| \) is the same as that of the parent bulk SC. However, the phase winding of the order parameter yields nontrivial phenomena. While the connection of \( \varphi_c(k) \) to the angle of the in-plane momentum \( \theta_k = \tan^{-1} k_y/k_x \) depends on the \( c_{ij} \) coefficients, the condition \( c_{xx}c_{yy} \neq c_{xy}c_{yx} \) guarantees that
\( \varphi_c(\mathbf{k}) \) always winds by \( 2\pi \) along any closed path around the \( \Gamma \)-point of the surface Brillouin zone. This is analogous to the case studied in Ref. [5] where Majorana fermions have been demonstrated to appear within TI-SC heterostructures involving helical TI surface states.

In the triplet case Eq. (2.4) implies that the proximity-induced pairing is sensitive to the detailed form of the interface Hamiltonian, and the shape of the proximity-induced gap generally differs from that of the parent SC. Even for a fully gapped bulk SC, it is possible to have nodal interface superconductivity. This is evident already for \( H_D(\mathbf{k}) \), where we obtain \( \Delta_D(\mathbf{k}) = -ie^{-i\theta} [d(\mathbf{k}) \times \hat{k}] \). For concreteness below we assume a tetragonal crystal symmetry for the parent superconducting material and classify \( d(\mathbf{k}) \) according to irreducible representations of the \( D_{4h} \) point group. For example, the fully gapped helical \( A_{2u} \) parent state \( d_{A_{2u}}(\mathbf{k}) = \Delta_0(\hat{k}_y \hat{x} - \hat{k}_x \hat{y}) \) leads to fully-gapped superconductivity in the TI layer, while the parent \( B_{1u} \) state \( d_{B_{1u}}(\mathbf{k}) = \Delta_0(\hat{k}_x \hat{x} - \hat{k}_y \hat{y}) \) and the parent \( B_{2u} \) state \( d_{B_{2u}}(\mathbf{k}) = \Delta_0(\hat{k}_y \hat{x} + \hat{k}_x \hat{y}) \) produce \( d \)-wave-like nodal gaps. This result is in agreement with the symmetry-based analysis of Ref. [26]. Deviations from the vector \( c_D(\mathbf{k}) \) introduce additional anisotropies into the proximity-induced gap. These reflect the lower symmetry due to interface potentials, but do not qualitatively change the gap structure.

Qualitative differences appear for triplet parent materials with \( A_{1u} \) or \( E_{2u}^+ \) pairing states, \( d_{A_{1u}}(\mathbf{k}) = \Delta_0(\hat{k}_x \hat{x} + \hat{k}_y \hat{y}) \) and \( d_{E_{2u}^+}(\mathbf{k}) = \Delta_0(\hat{k}_x \pm i\hat{k}_y) \hat{z} \), respectively. In both cases a conventional Dirac interface Hamiltonian yields no proximity-induced superconductivity [19, 26, 27]. In contrast, we find that a more general \( c(\mathbf{k}) \) reflecting the effects of the interface potentials enables pairing of the interface states. For the \( A_{1u} \) SC the induced superconducting order parameter may be nodal or fully gapped depending on the specific choice of \( c_{ij} \). Below, motivated in part by the studies of SrRu\(_2\)O\(_4\), we focus on the chiral \( E_{2u}^+ \) case and investigate signatures of symmetry breaking at the TI-SC interface in the proximity-induced superconductivity.
2.4. Interface Potentials and Proximity Effect With Chiral SCs

In this section we introduce a specific model for the $c_{ij}$ coefficients. As is evident from Eq. (2.4), the proximity effect for chiral $E_{2u}^+$ SCs requires $c_z(k) \neq 0$, leading to an induced gap that has nodes along the directions $c_{zx}k_x + c_{zy}k_y = 0$ in the interface plane. Although at vacuum terminations $H_D(k)$ has $c_z(k) = 0$, this coefficient is nonzero in the presence of interface scattering that breaks rotational symmetry in the plane of the interface [17].

Here we adopt results from the microscopic model of Ref. [17], which shows that if $u$ is the strength of a symmetry-breaking interface potential at the $z = 0$ interface, then the effective interface Hamiltonian is characterized by the coefficients

$$c_u(k) = \hbar v_F \left( k_y - \frac{k_x}{1 + G(u)}, -\frac{\sqrt{2G(u)}}{1 + G(u)} k_x \right)^T. \tag{2.5}$$

Here $G(u) = (u^2/G_0)/[1 + (u^2/G_0)^2] \leq 1$, where $G_0$ is a real parameter whose numerical value is determined by the material parameters of the heterostructure. This form for the interface Hamiltonian indeed breaks rotational symmetry, having an elliptical Fermi surface and with the $c_z(k) \neq 0$ term generating a rotation of the interface state’s spin out of the plane of the interface.

We thus expect that any interface scattering that breaks rotational symmetries will generally lead to an interface Hamiltonian characterized by Eq. (2.5), and now investigate its experimental implications. In the absence of interface potentials ($u = 0$) and for a strong barrier ($u^2 \gg G_0$), this expression recovers the helical Dirac case $c_D(k)$. The maximal deviation from $c_D(k)$, where we expect the strongest proximity effect, occurs at $u_{\text{max}} = \sqrt{G_0}$. In Fig. 2.1(a) we show the evolution of the proximity-induced order parameter for various values of the interface potential strength $u$. Since $G(u)$ is a slowly varying algebraic function of $u$ the eigenstates of the interface Hamiltonian, Eq. (2.1), retain a significant out-of-plane spin component and therefore allow for the proximity coupling to a chiral triplet, even for potential strengths far from $u_{\text{max}}$. 


Note that the constant energy surfaces for the interface Hamiltonian Eq. (2.1) with the choice of the coefficients in Eq. (2.5) are elliptical, elongated in the $k_x$ direction. The orthogonal choice of another symmetry-breaking interface potential gives the ellipse elongated along the $k_y$ axis. In general, however, the existence of $c_z(k)$ need not require ellipticity of the Fermi surface.

### 2.5. Conductance of Lateral Heterojunctions

Directly measuring the gap in the interface layer of a TI-SC heterostructure is technically difficult. Therefore we consider the signatures of the induced order parameter in the conductance of lateral heterojunctions, shown in Fig. 2.1(b), between region I with the usual vacuum-terminated TI surface defined by $c(k) = c_0(k)$ and region II with the TI-SC interface. To explore the salient consequences of the rotational symmetry breaking in the interface, we consider two simplified generic choices for the interface states, namely $c_{\parallel}(k) = \hbar v_F(k_y, -\lambda k_x, -\lambda k_x)^T$ and $c_{\perp}(k) = \hbar v_F(\lambda k_y, -k_x, -\lambda k_y)^T$. In the following we present the results for $\lambda = 2/3$ chosen such that $c_{\parallel}(k) = c_{u_{\text{max}}}(k)$, so that the major axis of the elliptical Fermi surface for $c_{\parallel}(k)$ [$c_{\perp}(k)$] is parallel to the $x$ ($y$) axis. Crucially, with these choices the gap nodes of the proximity-induced superconducting order parameter from the chiral parent SC are along the $k_x = 0$ direction for $c_{\parallel}(k)$ and along the $k_y = 0$ direction for $c_{\perp}(k)$, as shown in the insets of Figs. 2.2(b) and 2.2(d).

This difference is manifested in the conductance due to Andreev reflection at the lateral junction. We compute the conductance spectra using the semi-classical Andreev equations [28–31]. Correct boundary conditions at the junction are critical for the wave function matching in the Andreev approach. These boundary conditions are not trivial for effective Hamiltonians that are linear in momentum, as is well-known from studies of graphene edge states [32–34]. We model the lateral edge by setting $\Psi_I(0) = M\Psi_{II}(0)$. As shown in Appendix A, the matrix $M$ is determined from the requirement that the Hamiltonian for the lateral junction is Hermitian, i.e. conserves the probability current. If in addition the heterostructure preserves time-reversal symmetry, we find a one-parameter family of boundary
conditions described by

$$\mathcal{M}(\beta) = \sqrt{\frac{v}{v_F}} [\tau_0 e^{i\sigma_y \beta} + \frac{i\tau_x}{2\hbar v} (c_{xz}\sigma_z - c_{zx}\sigma_x)e^{-i\sigma_y \beta}].$$ \hspace{1cm} (2.6)$$

Here $\tau_i$ are the Pauli matrices in the electron-hole space as written in the basis of Eq. (2.2), and $v = (\sqrt{\sum_i c_{ix}^2 - c_{yx}})/2\hbar$ with $i = x, y, z$. In the spirit of the weak-coupling limit we derived $\mathcal{M}(\beta)$ in the normal state, and neglected any modification of it due to the emergence of proximity-induced superconductivity. The parameter $\beta$ thus encodes all possible scattering phenomena at the junction compatible with time-reversal symmetry and particle conservation, and accounts for the fact that we are working with an effective low energy Hamiltonian [35, 36].

In the Andreev approximation we solve for wave functions of the form $\Phi(\mathbf{r}) = e^{i\mathbf{k}_F \cdot \mathbf{r}} \times (\mathbf{U}(\mathbf{r}), 0, \mathbf{V}(\mathbf{r}), 0)^T$, as given in the basis of Eq. (2.3), where $\mathbf{k}_F$ is the Fermi momentum. From the BdG equation $\mathcal{H}\Phi(\mathbf{r}) = E\Phi(\mathbf{r})$, we obtain the Andreev equations for the envelope functions $U(\mathbf{r})$ and $V(\mathbf{r})$,

$$EU(\mathbf{r}) = -i v_F(\mathbf{k}_F) \cdot \nabla U(\mathbf{r}) + \Delta(\mathbf{r}, \mathbf{k}_F) V(\mathbf{r}),$$

$$EV(\mathbf{r}) = i v_F(\mathbf{k}_F) \cdot \nabla V(\mathbf{r}) + \Delta^*(\mathbf{r}, \mathbf{k}_F) U(\mathbf{r}).$$ \hspace{1cm} (2.7)$$

Here $v_F(\mathbf{k}_F) = (\partial \xi / \partial \mathbf{k})|_{\mathbf{k}_F}$ with $\xi(\mathbf{k}) = |c(\mathbf{k})| - \mu$ being the normal state energy dependent on whether we are in region I or II. We define $\Delta(\mathbf{r}, \mathbf{k}_F) = \Delta(\mathbf{k}_F) \Theta(x)$, where $\Delta(\mathbf{k}_F)$ is given by Eq. (2.4) and $\Theta(x)$ is the Heaviside step function. As seen in Fig. 2.1(b), the proximity-induced order parameter vanishes as $x < 0$ (region I) and is nonzero only in region II ($x > 0$).

Upon obtaining the wave functions, we transform back to the basis of Eq. (2.2) and match the solutions using the matrix $\mathcal{M}(\beta)$ as given by Eq. (2.6). We then consider an incoming incident electron in region I with momentum $\mathbf{k}_1 = (k_x, k_y)^T$ and in-plane angle $\theta_k$. At the boundary, the electron may be retroreflected as a hole with momentum $\mathbf{k}_1$, or specularly reflected as an electron with momentum $\mathbf{k}_2 = (-k_x, k_y)^T$. The wave function in region I is
then $\Psi_1(\mathbf{r}) = \Psi_{\text{inc}}^1(\mathbf{r}) + A\Psi_{\text{ref}}^1(\mathbf{r}) + B\Psi_{\text{ref}}^1(\mathbf{r})$. In region II, the incident electron can either be transmitted as an electron-like quasiparticle with momentum $\mathbf{k}_1 = (k'_x, k'_y)^T$, or a hole-like quasiparticle with momentum $\mathbf{k}_2' = (-k'_x, k'_y)^T$.

We then solve for the coefficients $A$ and $B$. For a fixed energy $E$, the transmission coefficient for electrical current [29, 31, 37] can be defined as $\sigma_S(E, \theta_k, \beta) = 1 + |A|^2 - |B|^2$. Normalizing to the normal state value, $\sigma_N$, the total dimensionless conductance is defined as [31, 37]

$$\sigma_T(E, \beta) = \frac{\int_{-\pi/2}^{\pi/2} \sigma_S(E, \beta, \theta_k) \cos \theta_k d\theta_k}{\int_{-\pi/2}^{\pi/2} \sigma_N(\beta, \theta_k) \cos \theta_k d\theta_k}. \quad (2.8)$$

As may be expected, quasiparticles at near normal incidence give a dominant contribution to the conductance. For our choice of $c_{\parallel}(\mathbf{k})$ these quasiparticles see the full gap, while for $c_{\perp}(\mathbf{k})$ such quasiparticles travel along near-nodal directions. Consequently, we expect the features associated with superconductivity to be much more prominent for the former case.

Fig. 2.2 shows precisely this behavior. The conductance for the $c_{\perp}(\mathbf{k})$ case rapidly, and almost linearly, decreases from the value near $\sigma_T \approx 2$ characteristic of Andreev reflection, while for $c_{\parallel}(\mathbf{k})$ the conductance retains a more typical shape with a decrease from $\sigma_T = 2$ to $\sigma_T \rightarrow 1$ at energies comparable with the amplitude of the interface superconducting gap. Notably, this feature is robust with respect to the variations of the boundary parameter $\beta$, and therefore provides an unmistakable experimentally accessible signature of the symmetry breaking at the TI-SC interfaces.

2.6. Discussion

There are two parts to our analysis. First, we derived the form of the proximity-induced order parameter for an arbitrary parent superconductor and any set of coefficients $c_{ij}$ characterizing the topological interface state, Eq. (2.4), and showed that symmetry breaking at interfaces may drastically alter superconductivity in the interface layer. The most dramatic changes relative to previously studied cases occur for triplet systems, where the existence and shape of the proximity-induced gap are controlled by the deviations from the helical
Figure 2.2. Conductance of a lateral heterojunction with a chiral parent SC according to Eq. (2.8). (a) and (b) [(c) and (d)] are for the TI-SC interface described by $c_{\parallel}(k)$ [$c_{\perp}(k)$]. The vectors $c_{\parallel}(k)$ and $c_{\perp}(k)$ describe different types of interface potentials (see text). The top row shows the color map as a function of the boundary parameter $\beta$ in Eq. (2.6), and the bottom row shows $\sigma_T$ for select values of $\beta$. The insets give the shape of the induced superconducting gap at the interface.
Dirac surface spectrum, $c_D(k)$. The second part of our analysis focused on the particular case of the proximity effect with a fully gapped chiral triplet superconductor, and found that the superconductivity in the interface layer exists whenever $c_z(k) \neq 0$, and is nodal. We demonstrated that Andreev spectroscopy of the lateral heterojunctions provides information on the nodal structure of the proximity-induced gap, and therefore tests for the presence of such symmetry breaking interface potentials. We also found that the qualitative structure of the spectra is independent of the details of the scattering at the lateral junction.

While some of our results were obtained within a specific model of the interface, they are based on symmetry considerations and therefore we expect them to remain qualitatively correct irrespective of the detailed origin of the symmetry breaking. Our classification of the superconducting chiral states was done for the tetragonal $D_{4h}$ symmetry, while the [111] (in the rhombohedral unit cell) plane of the prototypical Bi$_2$Se$_3$ and related topological insulators has the hexagonal $D_{6h}$ symmetry. To lowest order in $k$, however, this does not change the results for the chiral order parameter and therefore our results hold. Away from the Dirac point, higher-order momentum corrections due to hexagonal warping may result in the appearance of out-of-plane spin components of the interface states [38], but the corresponding contribution to the order parameter is smaller than the leading order effect discussed here, and leads to a subdominant sixfold modulation of the superconducting order parameter.

Here, we did not consider the odd-frequency pairing component generated by the proximity-induced coupling at non-magnetic topological insulator surfaces [26, 39]. These odd-frequency correlations can result in crossed Andreev reflections and typically manifest themselves within similar double-junction geometries [39–41]. We therefore believe that their inclusion would not affect our conclusions for the transmission across a single interface.\(^1\) In

\(^1\)For the edge states of two-dimensional TIs, Ref. [41] suggested that the odd-frequency component may affect the conductance in single-junction geometries but argued that this reflects the peculiarities of the two-dimensional system.
a broader context, our results pave the way for the targeted design of superconducting proximity-induced orders via interface engineering.
3.1. Introduction

Topological Insulators (TIs) are a class of materials which admit linearly dispersing surface states and preserve time reversal (TR) symmetry [15, 16]. At vacuum terminations these surface states are isotropic and perfectly helical, such that the total angular momentum of the propagating state is perpendicular to the direction of its linear momentum, and is confined within the plane of the termination. The common assumption is that at interfaces of TIs with other materials, the interface states of the TI exhibit these same properties. However, the local environment of the interfacial boundary is qualitatively different than that of a vacuum terminated surface, and the available set of symmetries which the interface states must obey is lower than that of the bulk TI material. Effects from charge redistribution, dangling bonds, and lattice mismatch can introduce TR-preserving interface potentials which lower the symmetry and consequently alter the spin structure of the surface states within the interface. These states have been shown to exhibit elliptical energy contours and non-helical spin-momentum locking [7, 17].

Material interfaces of TIs with superconductors (SCs) have been predicted to host Majorana zero modes [5]. These objects are self-annihilating anyons with properties which are vital for the fields of fault-tolerant quantum computing and quantum information [5, 18]. The appearance of these Majorana zero modes in TI-SC heterostructures comes as a consequence of the spin-orbit interaction in the TI surface state. However, the nature of the superconductivity and the properties of the Majorana zero mode are dependent on the spin structure at the interface. In Ref. [7] it was demonstrated that interface potentials between the TI and SC materials are necessary to observe proximity-induced superconductivity for several classes of parent SCs.

In this chapter we analyze the conductance signatures of lateral heterojunctions of TI-vacuum and TI-SC interfaces as shown schematically in Fig. 3.1. While the TI-vacuum
interface has perfectly helical surface states, interface potentials between the TI and SC materials result in non-helical interface states. These new states with their altered spin textures have different anisotropic Fermi velocities compared to the helical states, making the analysis of the junctions between them nontrivial. We investigate both the normal state conductance and the superconducting Andreev conductance signatures which come from non-helical spin textures. We analyze how the consequences of non-helical spin textures compare to mismatches of the chemical potential, and on the orientation of the elliptical Fermi surface. We then compare the differences of these signatures between both parent s-wave SCs and parent helical spin-triplet SCs.

3.2. Model of the Lateral Heterojunction

We first calculate the normal state conductance of the lateral heterojunction shown in Fig. 3.1. On the left half space, the TI vacuum interface is described by the massless Dirac Hamiltonian $H_D(k) = \hbar v_F(\sigma \times k)_z - \mu_L$. Here $k = (k_x, k_y)^T$ is the in-plane momentum, $\sigma = (\sigma_x, \sigma_y, \sigma_z)^T$ is a vector of Pauli matrices in spin-space, $v_F$ is the Fermi velocity, and $\mu_L$ is the chemical potential as $x < 0$. On the right half space, Ref. [17] demonstrated
that nonmagnetic interface potentials modify the form of the interface Hamiltonian. These potentials result in interface states with anisotropic elliptical energy dispersions, and with spin textures which point out of the plane of the interface. To describe the TI interface in the normal state, we write the most general linear in momentum Hamiltonian that is TR invariant. We therefore study the following Hamiltonian incorporating both regimes:

$$H(k) = \begin{cases} \hbar v_F(\sigma \times k)_z - \mu_L, & \text{for } x < 0 \\ c(k) \cdot \sigma - \mu_R, & \text{for } x > 0 \end{cases} \quad (3.1)$$

Here $c(k)$ is a three-dimensional vector with purely real components such that $c_i(k) = \sum_j c_{ij}k_j$, and $\mu_R$ is the chemical potential at $x > 0$. We see that the right half space Hamiltonian becomes equal to the left as $c_D(k) = \hbar v_F(k_y, -k_x, 0)^T$. In this model, we have that $c(k) = -c(-k)$. The form of this Hamiltonian is therefore identical to that of antisymmetric spin-orbit coupling in non-centrosymmetric metals, and whose consequences on superconductivity have been extensively studied [24, 25]. What is different however is that the usual quadratic energy term is absent, placing us in a regime of infinite spin-orbit coupling strength. Ref. [17] demonstrated that the presence of interface potentials between a TI and topologically trivial materials can be encoded into the choice of the $c_{ij}$ coefficients. This prescription is valid so long as the transmission between the TI and SC materials is low, so that the TI interface states are still well defined [22, 23].

3.2.1. Normal State Conductance

In this section we compute the conductance of the lateral heterojunction in the absence of superconductivity. The low-energy linear Hamiltonians of the left and right half spaces are only effective descriptions on length scales much wider than the width of the boundary region localized at $x = 0$ [35, 42–44]. The matching of the wave functions of the left and right half spaces is nontrivial, as the two Hamiltonians have different Fermi velocities. Due to the fact that we only have a linear description, the continuity of the total space wave
function is not assured. In general, we may write

\[ \psi_L(0, y) = \mathcal{M} \psi_R(0, y) \]  

(3.2)

for some matrix \( \mathcal{M} \). In order for this to be a valid boundary value relation for our system, and hence valid for all wave functions of the Hilbert space, \( \mathcal{M} \) must respect the hermiticity of the Hamiltonian \( H(k) \) expressed in Eq. (3.1). That is, if both \( \psi_1(r) \) and \( \psi_2(r) \) are wave functions for all \( x \) that belong to \( H(k) \) in Eq. (3.1), we must have that \( \langle \psi_1|H\psi_2 \rangle = \langle H\psi_1|\psi_2 \rangle \).

Because translational symmetry is broken in the \( x \)-direction, we write \( k_x \rightarrow -i \partial_x \). Inserting this into the hermiticity condition and integrating by parts, we find

\[-\hbar v_F \mathcal{M}^\dagger \sigma_y \mathcal{M} = \sum_i c_{i\sigma} \sigma_x.\]  

(3.3)

Here, \( \mathcal{M} \) is a matrix with four independent matrix elements. To explicitly solve for each element in \( \mathcal{M} \), it is necessary to restrict the form of \( \mathcal{M} \) by taking note that \( \mathcal{M} \) must respect the discrete symmetries of the system. Let \( \mathcal{T} = i \sigma_y K \) be the TR symmetry operator where \( K \) is complex conjugation, and let \( \psi \) be a wave function over all space such that

\[ \psi(r) = \begin{cases} 
\psi_L(r) & \text{for } x < 0 \\
\psi_R(r) & \text{for } x > 0
\end{cases}.\]  

(3.4)

Because the system preserves TR symmetry, we know that \( \mathcal{T}\psi \) is also a wave function of our system. The matrix \( \mathcal{M} \) holds for all wave functions in the Hilbert space, which implies both \( \psi_L(0, y) = \mathcal{M}\psi_R(0, y) \) and \( \mathcal{T}\psi_L(0, y) = \mathcal{M}\mathcal{T}\psi_R(0, y) \). However, by applying \( \mathcal{T} \) on the left of both sides of the first expression, we have \( \mathcal{T}\psi_L(0, y) = \mathcal{T}\mathcal{M}\psi_R(0, y) \). This demonstrates that \( [\mathcal{T}, \mathcal{M}] = 0 \). This condition implies that \( \mathcal{M} \) must take the form \( \mathcal{M} = \gamma_0 \sigma_0 + i(\gamma_x \sigma_x + \gamma_y \sigma_y + \gamma_z \sigma_z) \), where all the \( \gamma_i \) are purely real. With this restriction, Eq. (3.3) can be solved to explicitly find each component of \( \mathcal{M} \). As demonstrated explicitly in
Appendix A, we find

\[
\mathcal{M}(\beta) = \sqrt{\frac{v}{v_F}} \left[ e^{i\sigma_y \beta} + \frac{i}{2\hbar v}(c_{zx} \sigma_z - c_{xz} \sigma_x) e^{-i\sigma_y \beta} \right].
\]  (3.5)

Here \( v = (\sqrt{\sum_i c_{ix}^2} - c_{yx})/2\hbar \). We see that this matrix depends on one free parameter \( \beta \in [0, 2\pi) \).

We now solve the scattering problem at the \( x = 0 \) boundary to obtain the normal state conductance of the lateral heterojunction. We consider an incoming electron on the \( x < 0 \) side with momentum \( \mathbf{k}_1 = (k_x, k_y)^T \) and in-plane momentum angle \( \theta = \tan^{-1} k_y/k_x \), a reflected electron with momentum \( \mathbf{k}_2 = (-k_x, k_y)^T \), and a transmitted electron with momentum \( \mathbf{k}_1' = (k_x', k_y)^T \). All of these states are conduction band electrons on the Fermi surface. The outgoing angle \( \theta' \) may be solved for in terms of the incoming angle due to the conservation of normal state energy and the conservation of the \( k_y \) momentum. The wave function on the \( x < 0 \) side is given by

\[
\psi_L(r) = \frac{e^{i\mathbf{k}_1 \cdot r}}{\sqrt{2}} \begin{pmatrix} 1 \\ -i e^{i\theta} \end{pmatrix} + r \frac{e^{i\mathbf{k}_2 \cdot r}}{\sqrt{2}} \begin{pmatrix} 1 \\ i e^{-i\theta} \end{pmatrix}.
\]  (3.6)

On the \( x > 0 \) side the wave function is

\[
\psi_R(r) = r e^{i\mathbf{k}_1' \cdot r} \begin{pmatrix} \cos(\vartheta_{c(\mathbf{k}_1')/2}) \\ e^{i\varphi_{c(\mathbf{k}_1')}} \sin(\vartheta_{c(\mathbf{k}_1')/2}) \end{pmatrix}.
\]  (3.7)

Here \( \vartheta_{c(\mathbf{k}_1')}, \varphi_{c(\mathbf{k}_1')} \) are the polar and azimuthal angles of the vector \( \mathbf{c}(\mathbf{k}_1') \), respectively. Matching the wave functions at the \( x = 0 \) boundary by writing \( \psi_L(0, y) = \mathcal{M}(\beta)\psi_R(0, y) \), we can solve for the reflection coefficient \( r \) and define the normal state conductance as

\[
\sigma_N(\theta, \beta) = 1 - |r(\theta, \beta)|^2.
\]  (3.8)
Figure 3.2. Plot of the normal state conductance $\sigma_N(\theta, \beta)$ as both sides of the lateral heterojunction are described by $H_D(k)$. We see that $\beta$ acts as an angle-dependent scattering potential at the one dimensional interface between the right and left half spaces of the lateral heterojunction.
To demonstrate the consequences of \( \beta \) on normal state conductance, we analyze \( \sigma_N \) in the case that both the left and right half spaces are described by the same Hamiltonian \( H_D(k) \). When \( \beta \) is zero, the conductance is always unity. However, when \( \beta \) is nonzero, the conductance is modified. The most dramatic changes occur for \( \beta = \pi/2 \), which we plot in Fig. 3.2. We see that \( \beta \) acts as an angle-dependent scattering potential between the two planar regions localized at \( x = 0 \). Due to Klein tunneling, Dirac particles are incapable of back-scattering from normal incidence \( \theta = 0 \). This is reflected in Fig. 3.2. Regardless of the strength of any scattering potential located at \( x = 0 \), there will always be a nonzero amount of conductance due to Klein tunneling. We can thus see that the effects of interfacial scattering potentials can be encoded into the form of the boundary matching matrix \( M(\beta) \).

### 3.3. Superconducting Lateral Heterojunctions

To obtain the conductance of the superconducting lateral heterojunction, we analyze the system shown in Fig. 3.1. We can obtain the form of the proximity-induced order parameter by projecting the Cooper pair structure of the parent SC onto the eigenstates of the interface Hamiltonian. Writing \( (b_{k\uparrow}, b_{k\downarrow}) \) as the electron field operators and introducing the Nambu-spinor \( \Psi = (b_{k\uparrow}, b_{k\downarrow}, b_{-k\uparrow}^\dagger, b_{-k\downarrow}^\dagger)^T \), the Bogoliubov-de Gennes (BdG) Hamiltonian may be written as

\[
\mathcal{H} = \frac{1}{2} \sum_k \Psi^\dagger \begin{pmatrix} H(k) & \hat{\Delta} \\ \hat{\Delta}^\dagger & -H^T(-k) \end{pmatrix} \Psi. \tag{3.9}
\]

Here \( H(k) \) is given by Eq. (3.1), and for a parent \( s \)-wave SC on the \( x > 0 \) half space we have \( \hat{\Delta} = i\sigma_y \Delta_0 \Theta(x) \), where \( \Theta(x) \) is the Heaviside step function. Once again, matching the wave functions on the left and right half spaces of the BdG Hamiltonian is nontrivial. We can generally write

\[
\Psi_L(0, y) = \mathcal{M}_S \Psi_R(0, y) \tag{3.10}
\]

and solve for the matrix \( \mathcal{M}_S \) using the hermiticity of the BdG equation given in Eq. (3.9). Doing so, we find that \( \mathcal{M}_S \) is a block diagonal matrix such that the upper block is defined by \( H(k) \) and the lower block is defined by \( -H^T(-k) \). While the upper block has the form
\( \mathcal{M}(\beta) \) in Eq. (3.5), the lower block can be interpreted to be the boundary value matching condition for holes, and solving for its form gives the result \( \mathcal{M}^*(\beta) \), as the complex conjugate.

In the mean field BdG description, the Hamiltonian \( \mathcal{H} \) is written in a redundant formalism where the hole degrees of freedom are constructed from the electron Hamiltonian \( H(k) \). Because \( -H^T(-k) \) is not independent of \( H(k) \), we see that if \( \mathcal{M}(\beta) \) has a particular value for its free parameter \( \beta \), then \( \mathcal{M}^*(\beta) \) must also have this same value for its free parameter. This is due to the fact that we cannot introduce a new degree of freedom by simply writing a redundant description of the electron Hamiltonian \( H(k) \). The boundary value matrix for the BdG wave functions is then

\[
\mathcal{M}_S(\beta) = \begin{pmatrix} \mathcal{M}(\beta) & 0 \\ 0 & \mathcal{M}^*(\beta) \end{pmatrix}.
\] (3.11)

We can now obtain the BdG wave functions of the left and right half spaces from the Andreev approximation [28–31]. The Andreev approximation holds in the limit \( \mu \gg \Delta_0 \), such that only the conduction band approaches the Fermi surface. Writing \( a_k \) as the annihilation operator of the conduction band eigenstate of \( H(k) \), we obtain from the weak coupling limit

\[
\mathcal{H} \approx \frac{1}{2} \sum_k \Phi^\dagger \begin{pmatrix} \xi(k) & \Delta(k) \\ \Delta^*(k) & -\xi(k) \end{pmatrix} \Phi.
\] (3.12)

Here \( \Phi = (a_k, a_{-k}^\dagger)^T \), and \( \Delta(k) = -e^{-i\phi_c(k)} \Delta_0 \Theta(x) \). The normal state energy is given by \( \xi(k) = \hbar v_F |k| - \mu_L \) for \( x < 0 \) and is given by \( \xi(k) = |c(k)| - \mu_R \) for \( x > 0 \). In the basis of Eq. (3.12), the wave function of \( \mathcal{H} \) has the form \( \Phi(r) = (u(r), v(r))^T \). For a spatially inhomogeneous order parameter, the BdG equations are given by [30]

\[
Eu(r_1) = \xi u(r_1) + \int dr_2 \Delta(r_1, r_2)v(r_2),
\]

\[
Ev(r_1) = -\xi v(r_1) + \int dr_2 \Delta^*(r_1, r_2)u(r_2).
\] (3.13)
In the Andreev approximation, we write \( \Phi(\mathbf{r}) = e^{ik_F \cdot \mathbf{r}} (U(\mathbf{r}), V(\mathbf{r}))^T \), where \( k_F \) lies on the Fermi surface. From writing \( \mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2 \) and \( \mathbf{s} = \mathbf{r}_2 - \mathbf{r}_1 \) as the center of mass and relative coordinates respectively, and defining \( \Delta(\mathbf{R}, \mathbf{k}) = \int \Delta(\mathbf{R}, \mathbf{s}) e^{i\mathbf{k} \cdot \mathbf{s}} d\mathbf{s} \), and by writing \( \xi(k_F - i\nabla) \approx (\partial \xi / \partial k)|_{k_F} \cdot (-i\nabla) \), we arrive to the Andreev equations:

\[
EU(\mathbf{r}_1) = -i v_F(k_F) \cdot \nabla U(\mathbf{r}_1) + \Delta(\mathbf{r}_1, k_F) V(\mathbf{r}_1),
\]

\[
EV(\mathbf{r}_1) = i v_F(k_F) \cdot \nabla V(\mathbf{r}_1) + \Delta^*(\mathbf{r}_1, k_F) U(\mathbf{r}_1).
\]

Here \( v_F(k_F) = (\partial \xi / \partial k)|_{k_F} \), and \( \Delta(\mathbf{r}_1, k_F) = -e^{-i\varphi(k_F)} \Delta_0 \Theta(x) \). By solving the Andreev equations we can obtain the wave functions for our system. We can then solve the scattering problem to find the conductance of the superconducting lateral heterojunction. We consider an incoming incident electron on the \( x < 0 \) side with momentum \( k_1 \) and in-plane angle \( \theta \). At the boundary, the electron may be retroreflected as a hole with momentum \( k_1' \), or specularly reflected as an electron with momentum \( k_2 \). In the basis of Eq. (3.9), the wave function on the \( x < 0 \) side is given by

\[
\Psi_L(\mathbf{r}) = \frac{e^{i k_1^+ \cdot \mathbf{r}}}{\sqrt{2}} \begin{pmatrix} 1 \\ -ie^{i\theta} \\ 0 \\ 0 \end{pmatrix} + A \frac{e^{i k_1^- \cdot \mathbf{r}}}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ ie^{-i\theta} \end{pmatrix} + B \frac{e^{i k_2^+ \cdot \mathbf{r}}}{\sqrt{2}} \begin{pmatrix} 1 \\ ie^{i\theta} \\ 0 \\ 0 \end{pmatrix}.
\]

Note that we use this basis, as the basis of Eq. (3.12) is momentum dependent. Here \( k^\pm = (k^+_x, k_y)^T \), where \( k^+_x = k_x \pm E/v_F x(k) \). On the \( x > 0 \) side, the incident electron can either be transmitted as an electron-like quasiparticle with momentum \( k_1' \) and in-plane angle \( \theta' \), or a hole-like quasiparticle with momentum \( k_2' = (-k_x', k_y)^T \). The wave function on the
Here $N_{\pm}^{-1/2} = \Delta_0 / \sqrt{2E(\pm \sqrt{E^2 - \Delta_0^2})}$ and $f_{\pm}(k) = (E \pm \sqrt{E^2 - \Delta_0^2})/(-e^{-i\varphi(k)} \Delta_0)$. We have that $k^{t\pm} = (k_x^{t\pm}, k_y) T$ where $k_x^{t\pm} = k_x' \pm \sqrt{E^2 - \Delta_0^2}/v_{Fx}(k')$. We can then match the wave functions as $\Psi_L(0,y) = M_S(\beta)\Psi_R(0,y)$, and solve for the coefficients $A$ and $B$. We are then able to define the transmission coefficient for electrical current of the superconducting lateral heterojunction [29, 31, 37] as $\sigma_S(E,\theta,\beta) = 1 + |A|^2 - |B|^2$. From here, we can define the normalized conductance $\sigma_R(E,\theta,\beta) = \sigma_S/\sigma_N$, and the total conductance as

$$\sigma_T(E,\beta) = \frac{\int_{-\pi/2}^{\pi/2} \sigma_S(E,\theta,\beta) \cos \theta d\theta}{\int_{-\pi/2}^{\pi/2} \sigma_N(\theta,\beta) \cos \theta d\theta},$$

(3.17)

where $\sigma_N(\theta,\beta)$ is the normal state conductance given in Eq. (3.8).

### 3.4. Conductance Signatures

Having found the normalized and total conductances of the superconducting lateral heterojunction shown in Fig. 3.1, in this section we now analyze the consequences of nonhelical spin textures as encoded in the choice of the $c_{ij}$ coefficients. We first analyze the normalized conductance $\sigma_R$. In Fig. 3.3(a), we plot $\sigma_R$ in the case that $c(k) = c_D(k)$, so that both sides of the heterojunction admit helical surface states. When $\beta = 0$, there is no scattering at the junction, and all incoming angles $\theta$ experience perfect Andreev reflection for energies below
Figure 3.3. (a) Normalized conductance for several incoming angles for the superconducting lateral heterojunction, such that $c(k) = c_D(k)$ and $\beta = \pi/2$. (b) Total conductance of the superconducting lateral heterojunction such that $c(k) = c_D(k)$.

the gap edge. As $\beta = \pi/2$, we see that the probability of specular reflection due to scattering increases. However, we find that the normal incidence incoming angle always experiences perfect Andreev reflection, regardless of the strength of $\beta$. This is a direct consequence of Klein tunneling and the inability to confine Dirac particles. Like we observed in the normal state, we once again see that $\beta$ acts as an angle-dependent scattering potential. This highlights the intrinsic difference between Dirac and Schrödinger physics in superconducting junctions. While in conventional materials a boundary potential is able to completely suppress the normal state conductivity, this is never the case for Dirac electrons. The consequence of this in the Andreev conductance spectrum is that there will be no divergence in the total conductance at the gap edge, but rather a maximum. This can be seen in Fig. 3.3(b), where a maximum occurs at the gap edge for nonzero values of $\beta$. A transparent interface boundary occurs when $\beta$ vanishes, and the total conductance experiences perfect Andreev reflection for all incoming angles.
Figure 3.4. (a) Total conductance as \( c(k) = c_D(k) \). Here it can be observed that a mismatch in the chemical potentials can introduce a peak at the gap edge, but not as large as the consequences of the angle-dependent scattering potential controlled by \( \beta \) localized at the \( x = 0 \) boundary. (b) Total conductance of the superconducting lateral heterojunction in the case that the velocity on the \( x > 0 \) side is reduced, such that \( v_2 = 0.7v_F \).

In Fig. 3.4(a), we compare the effects of \( \beta \) to that of a mismatch of the chemical potential. While the chemical potential mismatch similarly creates a maximum in the total conductance at the gap edge, the effect is not as pronounced as that from \( \beta \). This demonstrates that scattering effects at the \( x = 0 \) boundary have a significant impact in the conductance signatures. In Fig. 3.4(b), we plot the total conductance in the case that the \( x > 0 \) side has a renormalized velocity, such that \( v_2 = 0.7v_F \). We can see that this mismatch of the velocities creates additional scattering in addition to the effects caused by \( \beta \).

It has recently been demonstrated that rotational symmetry breaking interface potentials present in TI heterostructures can introduce elliptical energy contours and out-of-plane spin textures in TI interface states. Two examples of such spin textures have been found to be modeled by \( c_{\perp}(k) = \hbar v_F(\lambda k_y, -k_x, -\lambda k_y)^T \) and \( c_{\parallel}(k) = \hbar v_F(k_y, -\lambda k_x, -\lambda k_x)^T \), where \( 0 < \lambda < 1 \) [7]. The first spin texture introduces an elliptical Fermi surface with a major axis which is perpendicular to the \( x \)-axis, while the second spin texture has an elliptical
Figure 3.5. (a) Total conductance in the case that $c(k) = c_\perp(k)$. (b) Total conductance in the case that $c(k) = c_\parallel(k)$. Here we have that $\lambda = 2/3$.

Fermi surface with a major axis parallel to the $x$-axis. In Fig. 3.5, we see that $c_\parallel(k)$ has the same total conductance spectrum as $c_D(k)$, while the total conductance of $c_\perp(k)$ is modified compared to the helical surface states. However, there are values of $\beta$ in which the scattering of the $x = 0$ boundary is reduced, and the system experiences perfect Andreev reflection for all incoming angles. While the direction of the ellipticity of the Fermi surface cannot be distinguished from the effects of $\beta$, we see that different ellipse directions require different values of $\beta$ to maximize the normal state conductance.

We also study the conductance signatures for several spin-triplet SCs. To analyze these systems, we must replace the order parameter of the parent SC on the $x > 0$ half of space in Eq. (3.9) with $\tilde{\Delta} = [d(k) \cdot \sigma](i\sigma_y)\Theta(x)$. Here the vector $d(k)$ represents the spin-triplet part of the pairing field. Carrying through a similar analysis as before, it has been shown in Ref. [7] that the proximity-induced order parameter of the TI-SC interface in Eq. (3.12) now takes the form $\Delta(k) = -e^{-i\varphi_\epsilon(k)}[\tilde{c}(k) \cdot d(k)]\Theta(x)$. For concreteness we assume a tetragonal crystal symmetry for the parent superconducting material and classify $d(k)$ according to the irreducible representations of the $D_{4h}$ point group. The conductance signatures of the
Figure 3.6. Total conductance for helical spin-triplet parent SCs in the case that $c(k) = c_D(k)$ for (a) a parent $A_{2u}$ SC (b) a parent $B_{1u}$ SC (c) a parent $B_{2u}$ SC.
chiral $E_{2u}^{\pm}$ pairing states in which $d_{E_{2u}^{\pm}}(k) = \Delta_0(\hat{k}_x \pm i\hat{k}_y)\hat{z}$ have been extensively studied in Ref. [7]. Below we focus on the helical $A_{1u}$, $A_{2u}$, $B_{1u}$, and $B_{2u}$ pairing states.

Assuming for the moment that $c(k) = c_D(k)$ and thus $\Delta_D(k) = -i e^{-i\theta} [d(k) \times \hat{k}]_z$, we find that the $A_{2u}$ pairing state with $d_{A_{2u}}(k) = \Delta_0(\hat{k}_y \hat{x} - \hat{k}_x \hat{y})$ produces isotropic fully gapped superconductivity at the interface. In contrast, the $B_{1u}$ pairing state with $d_{B_{1u}}(k) = \Delta_0(\hat{k}_x \hat{x} - \hat{k}_y \hat{y})$ and the $B_{2u}$ pairing state with $d_{B_{2u}}(k) = \Delta_0(\hat{k}_y \hat{x} + \hat{k}_x \hat{y})$ both produce $d$-wave-like nodal gaps. These differences manifest themselves in the Andreev conductance spectra plotted in Fig. 3.6.
For the $A_{1u}$ pairing state with $d_{A_{1u}}(k) = \Delta_0(\hat{k}_x\hat{x} + \hat{k}_y\hat{y})$, we find that there is no proximity-induced superconductivity as long as $c(k) = c_D(k)$. This shows that the proximity effect thus requires the presence of interface potentials in the TI-SC barrier which modify the spin texture of the interface state. In Fig. 3.7 we plot the total conductance for interface potentials described by $c_\perp(k)$ and $c_\parallel(k)$, respectively. In both cases we find that the conductance always obtains its largest value at zero energy, regardless of the scattering introduced by $\beta$. The orientation of the elliptical energy contours cannot be distinguished, as the effects from the interface scattering due to $\beta$ give rise to similar signatures. At energies comparable to the proximity-induced gap, the spectrum tends towards unity.

3.5. Discussion

In summary, we have developed a new analytical method to calculate the conductance of lateral Heterojunctions of TI interface states. While in conventional superconductors the tunneling conductance can be analyzed by the inclusion of a Dirac delta potential at the boundary, such potentials are intractable for linear effective models. This is because the evaluation-at-a-point behavior of Dirac delta potentials only applies to wave functions which are guaranteed to be continuous. Because the linear models of TI surface states do not guarantee continuity of the wave function, the tunneling conductance cannot be analyzed with such potentials. Our methods provide a means of analysis for linear Dirac Hamiltonians which are able to quantify the scattering at the boundary.

We then analyze the conductance signatures of superconducting lateral heterojunctions involving different spin textures for the TI interface states. In contrast to the conductance signatures in conventional superconductors, Dirac electrons only experience a maximum in the total conductance, as opposed to a divergence. The effects of $\beta$ are similar to the consequences of a mismatch in the chemical potentials, but more pronounced. We find that if the value of $\beta$ can be determined, the direction of elliptical Fermi surfaces of TI interface states can be determined from the conductance spectrum.
Chapter 4. Volkov-Pankratov States in Topological Superconductors

4.1. Introduction

Topological superconductors (TSCs) are materials which are predicted to host Majorana quasiparticles: excitations which behave as their own antiparticles [9, 16, 18, 45, 46]. These quasiparticles obey non-Abelian statistics, making them promising candidates for the topological qubits necessary for fault-tolerant topological quantum computation [47–49]. TSCs have been suggested to appear in a variety of condensed matter systems, including strong spin-orbit coupled semiconductor-superconductor (SC) hybrid devices [5, 50], fractional quantum Hall systems at filling factor $\nu = 5/2$ [51, 52], spinless $p_x + ip_y$ SCs [18], topological insulator-SC heterostructures [5, 7], integer quantum Hall insulators covered by conventional $s$-wave SCs [53], and thin films of transition metal dichalcogenides [54, 55].

Majorana zero modes (MZMs) are a zero-dimensional version of the Majorana quasiparticle that exist at strictly zero energy and are predicted to emerge at the ends of TSC nanowires and within TSC vortex cores [5, 11, 18]. While spectroscopic observations have provided promising signatures for their presence within these systems, it is difficult to energetically resolve the contributions from other effects such as Kondo correlations, Andreev bound states, weak antilocalization, and reflectionless tunneling [56–61]. Recent proposals have instead focused on one-dimensional (1D) realizations of Majorana quasiparticles known as chiral Majorana modes (CMMs), which can be found on the boundaries of two-dimensional (2D) TSCs. These CMMs are claimed to be responsible for the half-integer quantized conductance plateaus recently observed within quantum anomalous Hall insulator-SC hybrid structures, and have been predicted to be capable of performing quantum computational processes [62–64]. However, these claims are also under dispute as current research suggests that these half-quantized conductance plateaus can emerge from non-topological sources and are not predicated on the presence of CMMs within the system [65–67].

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Figure 4.1. (a) Schematic of a magnetic domain wall present in both a two-dimensional (top) and one-dimensional (bottom) SC. Band inversions occur when the energy gap $E_g = |B \pm \Delta|$ approaches zero (here $B$ is the Zeeman field and $\Delta$ is the SC gap). These band inversions define TPBs exhibiting Majorana quasiparticles, denoted by the dotted lines. (b) When the transition is sufficiently smooth, the spin-resolved LDOS becomes spin polarized due to the emergence of low-energy VP states, with opposite spin polarizations on either side of the TPB. The inset shows the linear spatial variation of the Zeeman exchange field.

that proper identification of MZMs and CMMs requires additional experimental signatures of their emergence.

In 1985 Volkov and Pankratov showed that semiconductor junctions with mutually inverted bands can result in the emergence of both massless states and massive states localized at the interface [68–74]. If the transition is sharp, only the massless state can be observed below the band gap of each material. In the language of topology, this massless state happens to be the topologically protected edge state whose existence is dictated by the bulk-edge correspondence underlying topological materials [16]. However, if the transition is sufficiently smooth massive states may also be observed. Junctions between topological and trivial materials, such as TSCs and SCs, result in similar band inversions which generate the Majorana bound state [13, 75–82]. The purpose of this chapter is then to study the properties of Volkov-Pankratov (VP) states which accompany band inversions in SCs with
smooth domain walls. Even though these massive states are not intrinsically topological, we stress that they appear as a consequence of the smooth transition between two SCs with different topological nature. While in this chapter we shall consider only magnetic domain walls, our predictions also apply to smooth transitions resulting from the variation of any other parameter controlling the topological index, such as the chemical potential.

We therefore demonstrate that smoothly varying band inversions generated by magnetic domain walls in both 1D and 2D SCs, schematically shown in Fig. 4.1 (a), generate massive states in addition to Majorana quasiparticles. In Sec. 4.2 we introduce a minimal model of an s-wave SC with Rashba spin-orbit coupling (SOC), where the band inversion is driven by a magnetic domain wall. We show that zero-energy Majorana excitations are accompanied by massive Volkov-Pankratov (VP) states whose energy gap is determined by the slope of the magnetic Zeeman exchange field associated with the domain wall. Furthermore, while the Majorana excitations are localized about the topological phase boundaries (TPBs) which are denoted by the dotted lines in Fig. 4.1, we show that the VP states split in real space away from these boundaries. We then analyze how the Majorana and VP states are affected by in-plane electric fields. Despite being electrically neutral, we show that their spatial positions may be controlled through the electric field strength. In addition, the energy level spacing of the VP states decreases as the electric field strength is increased. This is in line with the behavior of VP states in other topological materials, such as topological insulators [70, 83] or Weyl semimetals [72, 84], and finds its origin in the relativistic decrease of level spacings due to Lorentz boosts [85]. In Sec. 4.3 we calculate the spin-resolved Local Density of States (LDOS) in the vicinity of a TPB and apply these results to both a 1D nanowire and a 2D monolayer. We find that the VP states are spatially spin polarized with opposite polarizations on either side of the TPB, schematically shown in Fig. 4.1 (b). We predict this will be an observable signature through spin-resolved scanning tunneling spectroscopy measurements. In Sec. 4.4 we summarize our results and discuss the experimentally observable consequences of the VP states.
4.2. Model

In this chapter we analyze the emergence of VP states in two systems: a 1D nanowire and a 2D monolayer. Let us assume that both of these systems lie in the $x-y$ plane with a Zeeman exchange field $B(r)$ along the $z$-axis, as shown in Fig. 4.1. The normal state Hamiltonian for electrons with band mass $m$ in a monolayer system may be given by

$$H_{\text{layer}} = \left(-\frac{\nabla^2}{2m} - \mu\right)\sigma_0 + \alpha(\sigma \times -i\nabla)_z + B(r)\sigma_z. \quad (4.1)$$

Here and in the remainder of this chapter we use a system of units with $\hbar = 1$. The parameter $\alpha$ is the strength of the Rashba SOC, $\mu$ is the chemical potential, and $\sigma_i$ are the Pauli matrices in spin space. To model a nanowire, we may remove the degrees of freedom along the $x$-direction in the above Hamiltonian to obtain

$$H_{\text{wire}} = \left(-\frac{1}{2m}\partial_y^2 - \mu\right)\sigma_0 - i\alpha\partial_y\sigma_x + B(y)\sigma_z. \quad (4.2)$$

In this section we shall explicitly derive the solutions for the monolayer system, and note that the same techniques can equally be applied to $H_{\text{wire}}$. The Bogoliubov-de Gennes (BdG) Hamiltonian is then

$$\mathcal{H} = \frac{1}{2} \int dr \Psi^\dagger(r) H \Psi(r),$$

$$H = \left(-\frac{\nabla^2}{2m} - \mu\right)\tau_z\sigma_0 + B(r)\tau_z\sigma_z$$

$$+ \alpha(-i\partial_y)\tau_0\sigma_x - \alpha(-i\partial_x)\tau_z\sigma_y - \Delta\tau_y\sigma_y. \quad (4.3)$$

Here $\Psi(r) = (\psi_0(r), \psi_1(r), \psi_0^\dagger(r), \psi_1^\dagger(r))^T$ is the Nambu spinor with $\psi_\sigma(r)$ being the electron field operators, $\tau_i$ are the Pauli matrices for the particle-hole space of the BdG Hamiltonian, and $\Delta$ is the $s$-wave superconducting order parameter chosen to be real and positive. In the case that the magnetic field is homogeneous, such that $B(r) = B$, the energy spectrum of
this system has an energy gap at zero momentum given by

\[ E_g = \left| B \pm \sqrt{\Delta^2 + \mu^2} \right|. \tag{4.4} \]

For positive Zeeman exchange field, we see that the band gap closes at \( B = \sqrt{\Delta^2 + \mu^2} \). In the presence of a spatial variation in \( B \), there will be a topological phase transition from a Zeeman-dominated region \( (B > \sqrt{\Delta^2 + \mu^2}) \) to a pairing-dominated region \( (B < \sqrt{\Delta^2 + \mu^2}) \). Standard arguments based on topology show that the boundary between these regions shall lead to a CMM [11]. Here, we show that such a chiral Majorana state can be accompanied by additional massive VP states. To focus on the small momenta about the TPB, we neglect the kinetic energy term \( -\nabla^2/2m \) in our Hamiltonian and set \( \mu = 0 \) [86].

We observe that the band inversion is controlled by the Zeeman term \( B(r) \). In order to study a smooth interface between topological and trivial regions, we consider an exchange field profile localized around \( y = 0 \) and keep only the linear term in its Taylor expansion [11],

\[ B(y) = by. \tag{4.5} \]

Here the magnetic exchange field has a slope \( b > 0 \) and a characteristic length scale given by \( y_0 = \Delta/b \). To maintain the consistency of our low energy treatment, we shall later ensure that the localization length of the model’s bound states is smaller than \( y_0 \). We also note that, as discussed in Appendix B, the linear domain wall profile presented in Eq. (4.5) yields the same qualitative spectra as other choices of smoothly varying functions, such as \( \tanh(y) \) [73, 83].

### 4.2.1. Spectrum of the System

In the presence of an exchange field described by Eq. (4.5) our system exhibits two TPBs at \( \pm y_0 \), as shown by the dotted lines in Fig. 4.1. Our next task is then to find the low-energy Majorana and VP states near these positions. To see this in our model, we transform the
$4 \times 4$ matrix Hamiltonian of Eq. (4.3) using

$$U = \frac{e^{-i\pi/4}}{2} \begin{pmatrix}
-1 & 1 & -1 & 1 \\
-i & i & i & -i \\
i & i & -i & -i \\
1 & 1 & 1 & 1
\end{pmatrix}. \tag{4.6}$$

Since our system is translationally invariant along the $x$-direction, we write $\psi_\sigma(r) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \psi_{k\sigma}(y)$, where $k$ is the momentum along the $x$-direction and $L$ is the length of the system. These allow us to write our Hamiltonian in a more suggestive form,

$$\mathcal{H} = \frac{1}{2} \sum_k \int dy [U^\dagger \Psi_k(y)]^\dagger \times \begin{pmatrix}
-\alpha k & 0 & \sqrt{2\alpha} a_- & 0 \\
0 & -\alpha k & 0 & \sqrt{2\alpha} a_+ \\
\sqrt{2\alpha} a_- & 0 & \alpha k & 0 \\
0 & \sqrt{2\alpha} a_+ & 0 & \alpha k
\end{pmatrix} [U^\dagger \Psi_k(y)]. \tag{4.7}$$

Here $\Psi_k(y) = (\psi_{k\uparrow}(y), \psi_{k\downarrow}(y), \psi_{-k\uparrow}^\dagger(y), \psi_{-k\downarrow}^\dagger(y))^T$, and we have defined the ladder operators $a_\pm = \sqrt{\frac{\beta}{2\alpha}}[(y \pm y_0) + \frac{\alpha}{\beta} \partial_y]$. These are harmonic oscillator ladder operators defining states localized at $\mp y_0$, respectively. Using the easily obtained eigenvectors of Eq. (4.7), we can then obtain the following eigenvectors of the matrix Hamiltonian in Eq. (4.3) (within the
same approximations and with $-i\partial_x \rightarrow k$),

$$\varphi_{kn}^{-}(y) = UA_{kn}^{-} 
\begin{pmatrix}
\phi_{|n|}^{-}(y) \\
0 \\
Q_{kn}\phi_{|n|-1}^{-}(y) \\
0
\end{pmatrix},$$

$$\varphi_{kn}^{+}(y) = UA_{kn}^{+} 
\begin{pmatrix}
0 \\
0 \\
\phi_{|n|}^{+}(y) \\
Q_{kn}\phi_{|n|-1}^{+}(y)
\end{pmatrix}. \tag{4.8}$$

Here $n$ is an integer, and $\phi_{|n|}^{\pm}(y)$ are the Hermite functions which are eigenfunctions of the operators $a_{\pm}^{\dagger}a_{\pm}$ with eigenvalues $|n|$, given by

$$\phi_{|n|}^{\pm}(y) = \left( \frac{b}{\pi \alpha} \right)^{1/4} \frac{1}{\sqrt{2|n|!}} e^{-\frac{b}{2\alpha}(y \pm y_0)^2} H_{|n|} \left[ \sqrt{\frac{b}{\alpha}} (y \pm y_0) \right]. \tag{4.9}$$

Here $H_{|n|}(z)$ are the Hermite polynomials. We can see that these states are localized at $\pm y_0$, while the spatial extent of the wave functions are determined by the localization length $\ell = \sqrt{\alpha/b}$. The factors $A_{kn}$ and $Q_{kn}$ are given by

$$A_{kn} = \begin{cases} 
1, & n = 0 \\
\frac{1}{\sqrt{2}} \sqrt{\frac{2\alpha b|n|}{E_n(k)^2 + \alpha k E_n(k)}}, & n \neq 0
\end{cases}, \tag{4.10}$$

$$Q_{kn} = \begin{cases} 
0, & n = 0 \\
\frac{\alpha k + E_n(k)}{\sqrt{2\alpha b |n|}}, & n \neq 0
\end{cases}.$$
The energy eigenvalues of the BdG Hamiltonian are found to be

\[ E_n(k) = \begin{cases} 
-\alpha k, & n = 0 \\
\text{sgn}(n)\sqrt{(\alpha k)^2 + 2\alpha b|n|}, & n \neq 0 
\end{cases} \]  \hspace{1cm} (4.11)

This demonstrates that the CMMs \((n = 0)\), localized at \(\mp y_0\), are generically accompanied by massive VP states \((n \neq 0)\). As the transition becomes sharp, the parameter \(b\) increases and pushes the energy of the VP states above the superconducting gap \(\Delta\). Therefore, the VP states are only observable when the transition from non-magnetic to magnetic regions is sufficiently smooth. From the above expression we see that the first \((n = \pm 1)\) VP states enter the gap of the SC at the critical slope \(b_c = \Delta^2/2\alpha\), signaling the emergence of VP states into the system. We require that the localization length \(\ell\) be smaller than the TPB length scale \(y_0\), \(\ell \ll y_0\), which is equivalent to assuming \(\sqrt{\alpha b} \ll \Delta\). Indeed, one sees from Eq. (4.11) that this condition is equivalent to an energy of the first VP states begin below the bulk gap \(\Delta\). Otherwise, the VP states would simply not be visible.

To analyze the charge of the CMMs and VP states we calculate the expectation value of the charge operator \(\Xi = \text{diag}(e, e, -e, -e)\) with respect to \(\varphi_{kn}^\pm(y)\), where here \(e\) is the electron charge. A quick calculation shows that these expectation values are always zero for both the CMMs and VP states, implying that they are electrically neutral. As discussed in Ref. [87], this feature is a consequence of setting \(\mu = 0\).

To diagonalize the BdG Hamiltonian we set \(\Psi_k(y) = \sum_n (\varphi_{kn}^-(y)\gamma_{kn} + \varphi_{kn}^+(y)\beta_{kn})\) in Eq. (4.7) and obtain

\[ \mathcal{H} = \frac{1}{2} \sum_{kn} E_n(k)(\gamma_{kn}^\dagger\gamma_{kn} + \beta_{kn}^\dagger\beta_{kn}). \]  \hspace{1cm} (4.12)

Here \(\gamma_{kn}\) and \(\beta_{kn}\) are the annihilation operators for the bound states localized at \(+y_0\) and \(-y_0\) respectively. By expressing \(\gamma_{kn}\) and \(\beta_{kn}\) in terms of the electron field operators it can be shown that they each obey the relations \(\gamma_{kn}^\dagger = \gamma_{-k\cdot n}\) and \(\beta_{kn}^\dagger = -\beta_{-k\cdot n}\). When \(n = 0\) these expressions reduce to the Majorana criterion, according to which the Majorana
quasiparticle is identical to its own antiparticle [27]. We emphasize that Eq. (4.12) is a low-energy Hamiltonian, and that the summation over $n$ should only include those states that can be observed below the superconducting gap. From the form of $\Psi_k(y)$ we can express the electronic field operators in terms of the bound state ladder operators,

$$
\psi_{k\sigma}(y) = \sum_n \left( B_{kn\sigma}(y) \gamma_{kn} + C_{kn\sigma}(y) \beta_{kn} \right),
$$

$$
B_{kn\sigma}(y) = \begin{cases} \frac{e^{i\frac{5\pi}{4}}}2 A_{kn} [\phi_{n\downarrow}^-(y) + Q_{kn} \phi_{n\downarrow-1}^-(y)] & \sigma = \uparrow \\
\frac{e^{-i\frac{3\pi}{4}}}2 A_{kn} [\phi_{n\downarrow}^-(y) - Q_{kn} \phi_{n\downarrow-1}^-(y)] & \sigma = \downarrow 
\end{cases}, \quad C_{kn\sigma}(y) = \begin{cases} \frac{e^{i\frac{3\pi}{4}}}2 A_{kn} [\phi_{n\uparrow}^+(y) + Q_{kn} \phi_{n\uparrow-1}^+(y)] & \sigma = \uparrow \\
\frac{e^{-i\frac{\pi}{4}}}2 A_{kn} [\phi_{n\uparrow}^+(y) - Q_{kn} \phi_{n\uparrow-1}^+(y)] & \sigma = \downarrow 
\end{cases}
$$

(4.13)

If we then assume that the TPBs at $\pm y_0$ are sufficiently far apart such that $\phi_{n\uparrow}^\pm(\pm y_0) \approx 0$, in agreement with the condition that $\ell \ll y_0$, we may focus on the bound states localized at $+y_0$ by writing $\psi_{k\sigma}(y) \approx \sum_n B_{kn\sigma}(y) \gamma_{kn}$.

4.2.2. Effect of an in-Plane Electric Field

Next, we study the response of the CMMs and VP states under an in-plane electric field along the $y$-direction. To include this in our model, we introduce a spatially varying chemical potential into our Hamiltonian. The electric field is then given by the negative of the gradient of this potential. Still neglecting the kinetic energy term, the normal state Hamiltonian is then

$$
H_{\text{layer}} = -\mu(y) \sigma_0 + \alpha (\sigma \times -i \nabla)_z + B(y) \sigma_z.
$$

(4.14)

Here we define

$$
\mu(y) = my,
$$

(4.15)
Figure 4.2. Through the use of a hyperbolic transformation, the BdG Hamiltonian of Eq. (4.16) can be boosted into a frame in which the electric field vanishes. Whenever $|m| < b$, where $m$ is the electric field strength and $b$ is the slope of the Zeeman field, there exists a Lorentz boost along the black solid line into a frame in which $m = 0$. If instead $|m| > b$, there only exists a Lorentz boost along the dotted lines into a frame in which $b = 0$, removing the TPB and hence the CMM and VP states.
where \( m \) is the strength of the electric field which can either be positive or negative. The BdG Hamiltonian may then be written as

\[
\mathcal{H} = \frac{1}{2} \sum_k \int dy \Psi_k^\dagger(y) H \Psi_k(y),
\]

\[
H = -\mu(y) \tau_z \sigma_0 + B(y) \tau_z \sigma_z + \alpha (-i \partial_y) \tau_0 \sigma_x - \alpha k \tau_z \sigma_y - \Delta \tau_y \sigma_y.
\] (4.16)

As shown below, it is sufficient to consider the case \(|m| < b\). In this case we shall show that the BdG Hamiltonian may be transformed to a similar form as that of the previous section. To find the eigenvectors of the first quantized Hamiltonian such that \( H \phi = E \phi \), we apply a hyperbolic transformation that is akin to a Lorentz boost generated by \( \exp(\eta \tau_0 \sigma_z / 2) \), where \( \eta = \tanh^{-1}(m/b) \) [83, 84]. To perform this, we may rearrange the Schrödinger equation by writing

\[
\tilde{H} \tilde{\phi} = \gamma E \tilde{\phi}.
\] (4.18)

where here \( \mathcal{N} \) is a normalization constant included because the exponential matrices modify the norm of the wave function. As detailed in Appendix C, by rewriting the exponential matrices we may obtain the Lorentz-boosted Schrödinger equation,}

\[
\tilde{H} = \tilde{b} y \tau_z \sigma_z - \tilde{E} \tau_0 \sigma_z + \alpha (-i \partial_y) \tau_0 \sigma_x - \alpha k \tau_z \sigma_y - \Delta \tau_y \sigma_y.
\] (4.19)

Here \( \gamma = 1/\sqrt{1 - (m/b)^2} \) and \( \tilde{\phi} = \mathcal{N} e^{-\eta \tau_0 \sigma_z / 2} \phi \). We have also defined the Lorentz-boosted BdG Hamiltonian:

\[
\tilde{H} = \tilde{b} y \tau_z \sigma_z - \tilde{E} \tau_0 \sigma_z + \alpha (-i \partial_y) \tau_0 \sigma_x - \alpha k \tau_z \sigma_y - \Delta \tau_y \sigma_y,
\] (4.19)

where \( \tilde{b} = b/\gamma \) and \( \tilde{E} = \gamma \frac{m}{b} E \). Importantly, the spatially varying terms associated with \( \mu(y) \) are no longer present in \( \tilde{H} \). This Hamiltonian is then similar in form to the original.
BdG Hamiltonian in Eq. (4.3) of the previous section, with an additional constant term which depends on the energy. From the above expressions, we see that the behavior of this hyperbolic transformation is analogous to that of a Lorentz boost which transforms the electric field into a renormalized magnetic field, as shown in Fig. 4.2.

Recall that we assumed that $|m| < b$. If we instead had that $|m| > b$, we would be in the $m$-like quadrant of Fig. 4.2, and therefore would only be able to boost along the dashed line to a point with zero magnetic field ($b = 0$). Without any Zeeman exchange field, there will be no TPBs and therefore no CMMs nor VP states emerging within the system. This shows that if the electric field is too strong, the bound states are destroyed despite the fact that they are initially electrically neutral. In the following analysis we shall then assume that the slope of the chemical potential is sufficiently smooth such that $|m| < b$.

The similarity of Eq. (4.19) to Eq. (4.3) implies that we can find the low-energy CMMs and VP states via a similar approach. We then introduce the following energy-dependent unitary transformation

$$W_E = \frac{1}{2} \begin{pmatrix} -F_E^+ & F_E^- & -F_E^+ & F_E^- \\ -iF_E^+ & iF_E^- & iF_E^+ & -iF_E^- \\ iG_E^+ & iG_E^- & -iG_E^+ & -iG_E^- \\ G_E^+ & G_E^- & G_E^+ & G_E^- \end{pmatrix},$$

(4.20)

$$F_E^\pm = \frac{\pm \tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\sqrt{\tilde{E}^2 + \Delta^2 \pm \tilde{E} \sqrt{\tilde{E}^2 + \Delta^2}}},$$

$$G_E^\pm = \frac{\Delta}{\sqrt{\tilde{E}^2 + \Delta^2 \pm \tilde{E} \sqrt{\tilde{E}^2 + \Delta^2}}}.$$
This allows us to write our Lorentz boosted BdG Hamiltonian in a more suggestive form,

\[ W_E^\dagger H W_E = \begin{pmatrix}
-\alpha k & 0 & \sqrt{2ab\tilde{a}_-^\dagger} & 0 \\
0 & -\alpha k & 0 & \sqrt{2ab\tilde{a}_+^\dagger} \\
\sqrt{2ab\tilde{a}_-} & 0 & \alpha k & 0 \\
0 & \sqrt{2ab\tilde{a}_+} & 0 & \alpha k
\end{pmatrix}. \tag{4.21} \]

Here we have defined the ladder operators \( \tilde{a}_\pm = \sqrt{\alpha} \left[ (y \pm \sqrt{E^2 + \Delta^2}) + b \frac{2}{b} \partial_y \right] \). The similarity of Eq. (4.21) to Eq. (4.7) of the previous section allows us to quickly find the energy eigenvalues of the original Schrödinger equation,

\[ E_n(k) = \begin{cases}
-\frac{1}{\gamma} \alpha k, & n = 0 \\
\frac{1}{\gamma} \text{sgn}(n) \sqrt{(\alpha k)^2 + 2ab|n|}, & n \neq 0
\end{cases}. \tag{4.22} \]

The eigenvectors of \( H \) in Eq. (4.16) are then found to be

\[ \varphi_{n\pm}^\pm(y) = \frac{e^{\eta \alpha \sigma_z/2}}{N_{kn}} W_{E_n(k)} \tilde{A}_{kn} \begin{pmatrix}
\tilde{\phi}_{|n|}^- (y, k) \\
0 \\
\tilde{Q}_{kn} \tilde{\phi}_{|n|-1}^- (y, k) \\
0
\end{pmatrix}, \tag{4.23} \]

\[ \varphi_{n\pm}^\pm(y) = \frac{e^{\eta \alpha \sigma_z/2}}{N_{kn}} W_{E_n(k)} \tilde{A}_{kn} \begin{pmatrix}
0 \\
\tilde{\phi}_{|n|}^+ (y, k) \\
0 \\
\tilde{Q}_{kn} \tilde{\phi}_{|n|-1}^+ (y, k)
\end{pmatrix}. \]
Here, the Hermite functions $\tilde{\phi}^\pm_{|n|}(y, k)$ are once again the eigenfunctions of $\tilde{a}^\dagger \pm \tilde{a}^\pm$ with eigenvalue $|n|$, and are given by

$$\tilde{\phi}^\pm_{|n|}(y, k) = \left( \frac{\tilde{b}}{\pi \alpha} \right)^{1/4} e^{-\frac{\tilde{b}}{2\alpha} (y^\pm \sqrt{\frac{\tilde{E}_n(k)^2 + \Delta^2}{\tilde{b}}} \mp \frac{\alpha k}{\sqrt{2 \alpha \tilde{b} |n|}} \right)} H_{|n|} \left[ \sqrt{\frac{\tilde{b}}{\alpha}} \left( y^\pm \frac{\sqrt{\tilde{E}_n(k)^2 + \Delta^2}}{\sqrt{2 \alpha \tilde{b} |n|}} \right) \right].$$ (4.24)

The spatial location of the wave functions depends on the energy and electric field strength through $\tilde{E}_n(k) = \gamma \frac{m}{\tilde{b}} E_n(k)$, while their spatial extent now depends on the localization length $\ell = \sqrt{\alpha / \tilde{b}}$ which increases with the electric field strength. The terms $\tilde{A}_{kn}$ and $\tilde{Q}_{kn}$ are given by

$$\tilde{A}_{kn} = \begin{cases} 1, & n = 0 \\ 1 / \sqrt{2} \sqrt{\frac{2 \alpha k |n|}{\gamma E_n(k)^2 + \alpha k^2 E_n(k)}}, & n \neq 0 \end{cases}$$

$$\tilde{Q}_{kn} = \begin{cases} 0, & n = 0 \\ \alpha k + \gamma E_n(k) / \sqrt{2 \alpha \tilde{b} |n|}, & n \neq 0 \end{cases}.$$ (4.25)

From Eq. (4.22) we notice that the CMM, given by $n = 0$, still remains at zero energy despite the modification of its wave function by the electric field. We may observe that the effect of the electric field, regardless of its direction, is to shift the location of the bound states which are now localized at $y = \mp \sqrt{\tilde{E}_n(k)^2 + \Delta^2 / \tilde{b}}$. This amounts to spatially pushing apart the two TPBs. As shown in Fig. 4.1 (a) the region between the two TPBs, denoted by the dotted lines, is topologically trivial. When $|m| = b$, the entire system is then covered by the topologically trivial domain.

Using the wave functions in Eq. (4.23) we may similarly diagonalize the BdG Hamiltonian as in the previous section. However, in this case the $B_{kn\sigma}(y)$ and $C_{kn\sigma}(y)$ coefficients along with the $N_{kn}^\pm$ normalizations no longer have closed form analytic solutions, and must be
evaluated numerically. In addition, from Eq. (4.23) we may numerically calculate that the wave functions are no longer electrically neutral at \( m \neq 0 \).

### 4.3. Experimental Consequences

#### 4.3.1. Local Density of States

We have shown that the CMMs occurring in TPBs can be generically accompanied by low-energy VP states. Our next task is then to determine signatures of the VP states in the LDOS that is measurable via tunneling spectroscopy. We may determine the LDOS from the spectral function of the system. In the following we focus on the states localized at \(+y_0\) under the assumption that \( \ell < y_0 \). From the Fourier transform of the electronic retarded Green’s function \( G_R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -i\theta(t - t') \langle \{ \psi_\sigma(\mathbf{r}, t), \psi_{\sigma'}^\dagger(\mathbf{r}', t') \} \rangle \), with \( \theta(t) \) the Heaviside step function, we find the spectral function \( A(\mathbf{r}\sigma; \omega) = -2\text{Im}G_R(\mathbf{r}\sigma, \mathbf{r}\sigma; \omega) \) and thus the spin resolved LDOS as

\[
\rho_\sigma(\mathbf{r}, \omega) = \frac{A(\mathbf{r}\sigma; \omega)}{2\pi} = \frac{1}{L} \sum_{k n} |B_{k n \sigma}(y)|^2 \delta(\omega - E_n(k)).
\]  

(4.26)

The total LDOS \( \rho(\mathbf{r}, \omega) \) is then given as the summation of both spin components. We may then analyze both the 1D nanowire and 2D monolayer systems originally shown in Fig. 4.1.

#### 4.3.2. 1D Nanowire

Applying the techniques of the previous section to the case of a 1D nanowire, we find a discrete energy spectrum given by \( E_n = \frac{\text{sgn}(n)}{\gamma} \sqrt{2\alpha\tilde{b}|n|} \), which describes a set of MZMs and additional VP states localized at \( y = \pm \sqrt{\tilde{E}_n^2 + \Delta^2/\tilde{b}} \). Motivated by recent experiments, we set \( \Delta = 0.3 \text{ meV}, \alpha = 0.1 \text{ meV nm}, \) and \( b = 0.1 \text{ meV nm}^{-1} \) [13]. The superconducting coherence length of the system is then \( \xi = \alpha/\Delta \approx 0.33 \text{ nm} \). In this case we find that \( y_0 = 3 \text{ nm} \) and \( \ell = 1 \text{ nm} \), which maintains the consistency of the low-energy treatment introduced in Eq. (4.5).
Figure 4.3. Evolution of the nanowire bound state energies as the electric field strength is increased. Here \( m \) is the strength of the electric field and \( b \) is the slope of the Zeeman field. The MZM is denoted by the red dashed line, while the VP states are denoted by the blue solid lines. While the MZM remains at zero energy, the energy level spacing of the VP states decreases with increased electric field strength relative to the magnetic field slope.

In Fig. 4.3 we plot the energy spectrum of the nanowire bound states as a function of the electric field strength. We observe that as the electric field increases, there is a decrease in the energy level spacing of the MZM and VP states, and that more VP states emerge below the superconducting gap.

As \( \ell < y_0 \), we find that the two sets of bound states localized at \( \mp y_0 \) do not overlap in space, and may focus our analysis on the \( +y_0 \) states. The LDOS of the bound states centered at \( y_0 \) is given by \( \rho(y, \omega) = \sum_\sigma |B_{n\sigma}(y)|^2 \delta(\omega - E_n) \), where here \( B_{n\sigma}(y) \) is found by setting \( k = 0 \) in Eq. (4.13). In Fig. 4.4 we plot \( |B_{n\sigma}(y)|^2 \) for the MZM and first three positive VP states for \( m = 0 \). While the MZM is centered at the TPB, the VP states begin to split in space away from the phase boundary. In addition, while the MZM is not spin polarized, we see that the VP states are strongly spin polarized in space, with opposite spin polarizations on either side of the TPB. We find that these spin polarizations are interchanged for the \( n < 0 \) states.

In Fig. 4.5 we demonstrate the effect of the electric field on the bound states by numerically calculating the \( B_{n\sigma}(y) \) coefficients as discussed in Sec. 4.2.2. Regardless of the electric field direction, all of the states are shifted spatially to the right. This shift is easily seen.
Figure 4.4. Magnitude of the $B_{n\sigma}(y)$ coefficients which appear in the LDOS for the $n = 0, 1, 2, 3$ nanowire bound states in the absence of an electric field, shown in figures (a), (b), (c), and (d), respectively. The vertical black lines mark the TPB at $y_0 = 3$ nm. The dotted black lines denote the sum of both spin components. The MZM ($n = 0$) state is localized at $y_0$, while the VP ($n \neq 0$) states split away from the TPB, with opposite spin polarizations on either side.
Figure 4.5. Magnitude of the $B_{n\sigma}(y)$ coefficients in the presence of an electric field. Figures (a) and (b) show the MZM ($n = 0$) state as $m = b/2$ and $m = -b/2$ respectively, where $m$ is the strength of the electric field and $b$ is the slope of the Zeeman field. Figures (c) and (d) show the $n = 1$ VP state as $m = b/2$ and $m = -b/2$ respectively. The vertical black line marks $y_0 = 3$ nm, which is the topological phase boundary as $m = 0$. The insets in (c) and (d) show the orientation of the electric and magnetic fields as $m$ is positive and negative, respectively.
Figure 4.6. Energy spectrum of the monolayer bound states, where $k$ is the momentum along the $x$-direction and $\xi$ is the superconducting coherence length. The electric field is given by $m = 0$ and $m = b/2$ in figures (a) and (b) respectively, where $m$ is the strength of the electric field and $b$ is the slope of the Zeeman field. More VP states (blue solid lines) are introduced as the electric field strength increases, and the slope of the CMM is renormalized (red dashed lines).

through the TPB location $y = \sqrt{\tilde{E}_n^2 + \Delta^2/\tilde{b}}$, which acquires an energy-dependent displacement as a consequence of the Lorentz boost. In addition, the localization length increases with increasing field strength, causing the states to spread out in space. At $|m| = b$, we see that all of the states vanish as the localization length diverges. The spin polarization, however, depends on both the strength and direction of the electric field and are no longer equal and opposite in space.

4.3.3. 2D Monolayer

To analyze the case of a 2D monolayer, we adopt the parameter values of the previous section and plot the dispersion of Eq. (4.22) in Fig. 4.6. In contrast to the nanowire, this system exhibits a CMM which linearly disperses only in one direction parallel to the $x$ axis. Similar to the nanowire case, however, more VP states enter the gap as the electric field strength increases.

To evaluate the LDOS in Eq. (4.26) we convert the sum over momentum into an integral which we solve analytically and plot in Fig. 4.7 as a function of position and energy. Here
Figure 4.7. (a) Total LDOS of the monolayer system in the absence of an electric field, plotted as a function of position and energy. Here $\Delta = 0.3$ meV is the SC gap, and $y_0 = 3$ nm is the distance of the CMM to the center of the magnetic domain wall. The solid black and dashed red lines of constant position at $y_0$ and $1.5y_0$ are individually plotted in Figure (b). The LDOS is constant at low energies due to the linear dispersion of the CMM, while the peaks arise from the VP states. (c) Spin-up component of the spin-resolved LDOS. Lines of constant position are similarly plotted in Figure (d).
Figure 4.8. (a) Spin-up component of the spin-resolved LDOS of the monolayer system in the presence of an electric field given by $m = b/2$, where $m$ is the strength of the electric field and $b$ is the slope of the Zeeman field. Here $\Delta = 0.3 \text{ meV}$ is the SC gap, and $y_0 = 3 \text{ nm}$ is the distance of the CMM to the center of the magnetic domain wall in the absence of an electric field. The solid black and dashed red lines of constant position at $y_0$ and $1.5y_0$ are individually plotted in Figure (b). (c) Spin-down component of the spin-resolved LDOS. Lines of constant position at $y_0 \text{ nm}$ and $0.5y_0 \text{ nm}$ are individually plotted in Figure (d). The spin-up component is amplified, while the spin-down component is suppressed.
the LDOS creates an “X-shape” as a 2D manifestation of what was observed in Fig. 4.4 of the nanowire. For low energies, we see that the spectrum is constant due to the linear dispersion of the CMM localized at $y_0$. However, as the energy approaches the beginning of the VP bands, we see that the LDOS has large peaks which split in space about the TPB.

We note that the “X-shape” of these peaks in Fig. 4.7 (a) resembles what is experimentally observed in Ref. [13], in which magnetic Co-Si islands are deposited beneath a superconducting Pb monolayer. These Co-Si islands create a spatially varying Zeeman exchange field below the 2D SC, leading to a TPB on their circular edge which hosts CMMs. However, the experimental data unexpectedly displayed additional states apart from the CMM, splitting in space away from the Co-Si edge with nonzero energies. The LDOS above the Co-Si island is plotted in Fig. 2 (g) of Ref. [13] as a function of position and energy, and these additional states create an “X-shape” that is similar to what is analytically derived in Fig. 4.7 (a). We propose that the additional states observed in Ref. [13] are in fact VP states which emerge due to the smoothly varying exchange field decaying away from the Co-Si island.

To prove that the additional states found in Ref. [13] are truly VP states, we may analyze the spin-resolved LDOS in Fig. 4.7 (c). We find that the spin-up components are largely grouped to the right (left) of the TPB for positive (negative) energy values. The spin-down components are opposite, and are grouped on the left (right) of the TPB for positive (negative) energies. This shows that the spin-up and spin-down components of the VP states shift away from each other in space. These spin-polarizations can be measured via spin-resolved scanning tunneling spectroscopy experiments, and would provide additional evidence that the additional states observed in Ref. [13] are indeed VP states [88]. In our treatment we find that the CMM has equal spin-up and spin-down components, and is therefore not spin-polarized. This is a consequence of our $\mu = 0$ assumption, and in general the CMM may exhibit a net spin-polarization for nonzero values of the chemical potential [87]. In contrast, we expect that the strong spin-polarizations of the VP states
will be insensitive to small variations of the chemical potential, leading to easily identifiable signatures in spin-resolved scanning tunneling spectroscopy experiments.

In order to study the LDOS under the presence of an electric field, we once again convert the momentum summation of Eq. (4.26) into an integral which we evaluate analytically, and then numerically calculate the $B_{knσ}(y)$ coefficients as discussed in Sec. 4.2.2. In Fig. 4.8 we plot the spin-up and spin-down components of the LDOS once again as functions of position and energy. Similar to the previous section we find that for $m > 0$ the spin-up component is significantly amplified for positive energies, while the spin-down component is suppressed for negative energies. In the case that $m < 0$, however, we find that the spin-down component is amplified for negative energies, while the spin-up component is suppressed for positive energies. In addition, we see that all the bound states move to the right for all nonzero energy values, and that many more peaks appear in the LDOS due to the presence of additional VP states.

4.4. Conclusion

In this chapter we analyzed smooth magnetic domain walls that generate band inversions within 1D and 2D SCs. It is known that band inversions in 1D superconducting nanowires exhibit MZMs fixed at zero energy, while band inversions in 2D superconducting monolayers lead to linearly dispersing CMMs. While modern proposals have focused on CMMs as a potentially more robust alternative to the MZM for topological quantum computation, both MZMs and CMMs have been difficult to experimentally verify [62–67]. We have shown that if the transition between topological and trivial regions is smooth enough, the massless Majorana quasiparticles are accompanied by massive VP states. These VP states arise purely as a consequence of the transition between topologically different phases. While in this chapter we have focused on magnetic domain walls, we emphasize that our predictions equally apply to any other smooth transition that results from the variation of a parameter controlling the topological phase.
We have shown that the energy level spacing of the VP states is controlled by the slope of the Zeeman exchange field, and that the VP states are only observable below the superconducting gap when the slope of the exchange field is smaller than a critical value. We also found that while the Majorana states are localized at the TPB, the VP states split in space away from the TPB. In the case of a 2D monolayer, the splitting of the VP states creates an “X-shape” in the LDOS as a function of position. This X-shape is similar to what is experimentally observed in 2D SCs around spatially extended magnetic Co clusters, and we predict that VP states may be present within these systems [13]. We calculated how the VP states respond to in-plane electric fields, and have shown that their energy-level spacing depends on the electric field strength. As the strength of the electric field is increased, more VP states are observable below the superconducting gap. We also found that the spatial location of both the Majorana and VP states is controlled by the magnitude of the electric field. If the electric field becomes too strong, both the Majorana and VP states are destroyed as the entire system enters the trivial regime.

We derived the spin-resolved LDOS of the Majorana and VP states in the vicinity of a TPB. In contrast to the Majorana quasiparticles, we have found that the VP states are strongly spin polarized. As the VP states split in space away from the TPB, we have shown that opposite sides of the TPB display opposite spin polarizations. The magnitude of these spin polarizations is dependent on both the strength and direction of the electric field. In the case of zero field, the magnitudes of the spin polarization are equal and opposite on either side of the TPB, while nonzero electric fields lead to an asymmetry of these magnitudes across the TPB. We predict that this will be an observable signature of the VP states via spin-resolved scanning tunneling spectroscopy.
Chapter 5. Probing the Chirality of 1D Majorana Edge States Around a 2D Nanoflake in a Superconductor

5.1. Introduction

The quest for the realization of Majorana zero modes (MZMs), driven by the pursuit of both fundamental physics and their potential application to fault-tolerant topological quantum computation [46, 47, 49, 90, 91], is steering an active research in engineering $p$-wave superconductivity. Non-Abelian braiding is an essential step towards topological quantum computing, though it has not yet been experimentally achieved with MZMs. Due to the localized nature of MZMs, their braiding will necessarily involve both coupling and manipulation processes.

However, it has been suggested that non-Abelian braiding is not only restricted to MZMs, but can also be implemented with one-dimensional (1D) chiral Majorana fermions [64]. Chiral Majorana fermions can manifest themselves as quasiparticle edge states of a two-dimensional (2D) topological $p$-wave superconductor [16, 46]. Signatures of 1D chiral Majorana quasiparticles have been recently observed in 2D heterostructures consisting of a quantum anomalous Hall insulator bar in contact with a superconductor [62]. Additionally, recent progress in atomic scale engineering [13, 14, 92–94] is opening up new perspectives for the practical implementation of chiral Majorana fermions by spatially building non–trivial topological phases separated from trivial ones. Recent progress includes Co islands grown on a Si substrate and covered by a monolayer of Pb [13] and nano-scale Fe islands of monoatomic height on a Re surface [76]. Due to the non–trivial topological phase transition resulting from a gap closure, in-gap edge states surrounding the topological superconducting (SC) domain are observed. In both experiments, these in-gap states are strongly delocalized around the islands and have been interpreted as signatures of chiral Majorana fermions.

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Figure 5.1. (a) Schematic representation of the topological phase diagram as a function of the chemical potential $\mu$ and a magnetic Zeeman energy $h$. (b) Schematic view of the studied system. A superconducting (SC) layer (yellow transparent atoms) is deposited on a magnetic substrate (gray atoms). The nanoflake is formed by non-magnetic atoms located at random sites either between the substrate and the SC layer as shown in the figure or above the SC layer. For a constant SC gap $\Delta$, the boundary between the topologically trivial (blue region) and non–trivial phase (yellow region) is given by a parabola $h_c^2 = \Delta^2 + \mu^2$ [orange line in (a)].

In 2D superconductors with Rashba spin–orbit coupling (SOC), the transition to a non–trivial phase can be induced by an external Zeeman magnetic field [95–97]. The boundary between the trivial and non–trivial topological phases is given by $h_c^2 = \mu^2 + \Delta^2$, see Fig. 5.1(a), where $h_c$ stands for the critical Zeeman field for given values of the doping $\mu$ and the SC gap $\Delta$. In the aforementioned experimental results, the Zeeman magnetic energy arises from the presence of magnetic dopants interacting with the substrate, while the SOC and the SC gap are intrinsic to the subsystem. Looking at the phase diagram presented in Fig. 5.1(a), one observes that a line which connects the points A and B in the $(\mu, h)$ plane could correspond to an inhomogeneous system in real space, where a non-magnetic trivial domain (point A) surrounds or borders with a topological magnetic domain (point B).

In this chapter, we instead choose to explore an alternative route. We consider an inhomogeneous system but in a constant magnetic Zeeman energy, which would reside on the C–D line in Fig. 5.1(a). The transition to the topological domain occurs due to a change in the chemical potential $\mu$. Such a system could be constructed experimentally in many different ways: one option would be to substitute the magnetic atoms in the Co island [13] by non-magnetic ones and add a magnetic field parallel to the SC Pb monolayer [Fig. 5.1(b)].
Another promising approach is to use the versatility offered by 2D van-der-Waals heterostructures [98]. A possible way to generate an homogeneous Zeeman exchange energy in the proximity of a superconductor could be engineered by stacking recently synthesized 2D magnetic materials [99, 100] with a transition metal dichalcogenide (TMD) superconductor such as NbSe$_2$. A non-magnetic island can be obtained by evaporating some alkaline adatoms to enforce charge transfer.

In this chapter we start with a circular geometry for the nanoflake and derive the dispersive chiral Majorana edge states analytically in the continuum limit. We also discuss the spatial extent of the chiral Majorana modes in the tranverse direction.

5.2. Nanoflake With Circular Geometry

We begin by considering a nanoflake with a circular symmetry as depicted in Fig. 5.2. For simplification and without a loss of generality, we can also assume a smooth boundary of the nanoflake. Keeping in mind the circular symmetry, the Hamiltonian will commute with the $z$th component of the total angular momentum operator $J_z \equiv L_z + S_z$. We may then find the energies of the bound state wave functions localized at the edge of the nanoflake in terms of the $m_J$ quantum numbers. This method allows us to determine the existence of chiral subgap states within our system, and has successfully been used in the studies of other 2D systems with circular symmetry such as graphene [101].

Thus, the real-space normal state Hamiltonian has the form,

$$ H(r, \nabla) = \left( -\frac{\nabla^2}{2m} - \mu(r) \right) \sigma_0 + \alpha(\sigma \times -i\nabla)_z + h\sigma_z, $$

(5.1)

where $\sigma_i$ (for $i = \{0, x, y, z\}$) are the Pauli matrices acting in spin space. Here and in the remainder of this chapter we use a system of units with $\hbar = 1$. The system is 2D with
\( \mathbf{r} \equiv (x, y) \), and the chemical potential is given by,

\[
\mu(r) = \begin{cases} 
\mu_1 & r < R_0, \\
\mu_2 & r \geq R_0.
\end{cases}
\]  

(5.2)

We may also define the discontinuity \( \delta \mu = \mu_2 - \mu_1 \) at the boundary, see Fig. 5.2. In other words, \( \delta \mu \) corresponds to the spatial variation of the chemical potential induced by the nanoflake. The BdG Hamiltonian may then be expressed as,

\[
\mathcal{H} = \frac{1}{2} \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \begin{pmatrix} H(\mathbf{r}, \nabla) & i\sigma_y \Delta \\ -i\sigma_y \Delta & -H^T(\mathbf{r}, -\nabla) \end{pmatrix} \Psi(\mathbf{r}),
\]

(5.3)

where \( \Psi(\mathbf{r}) \equiv (\psi_\uparrow(\mathbf{r}), \psi_\downarrow(\mathbf{r}), \psi_\uparrow^\dagger(\mathbf{r}), \psi_\downarrow^\dagger(\mathbf{r}))^T \) is the Nambu spinor, with \( \psi_\sigma(\mathbf{r}) \) being electron field operators which destroy an electron with spin \( \sigma \) at location \( \mathbf{r} \).

Due to the circular symmetry of the nanoflake (or more precisely, the scalar chemical potential \( \mu(\mathbf{r}) = \mu(r) \)), the BdG Hamiltonian commutes with the \( z \)th component of the total angular momentum operator \( J_z = L_z + S_z \). It follows that the Hamiltonian and \( J_z \) share the same eigenstates. The eigenstates of \( J_z \), with the half-integer eigenvalues \( m_J \), are

![Figure 5.2](image.png)

Figure 5.2. Schematic representation of the discussed system with a circular nanoflake deposited on a substrate. The nanoflake locally modifies the systems chemical potential such that as \( r < R_0 \) (\( r > R_0 \)), the chemical potential is given by \( \mu_1 \) (\( \mu_2 \)). Given that \( \mu_1 \neq \mu_2 \) and under the presence of a constant magnetic exchange field, we find that chiral Majorana modes will emerge on the \( r = R_0 \) boundary.
given by

\[
\varphi_m = \begin{pmatrix}
    u_m^+(r) e^{i(mJ-\frac{1}{2})\theta} \\
    u_m^-(r) e^{i(mJ+\frac{1}{2})\theta} \\
    v_m^+(r) e^{i(mJ+\frac{1}{2})\theta} \\
    v_m^-(r) e^{i(mJ-\frac{1}{2})\theta}
\end{pmatrix}
\]

(5.4)

To focus on states with small total angular momenta, we take a low-energy approximation and neglect the kinetic energy term in the Hamiltonian [11]. By writing the \( u_{m\sigma}(r) \) and \( v_{m\sigma}(r) \) functions in terms of the modified Bessel functions of the first and second Kind, we may then solve for the bound state wave functions localized at \( r = R_0 \). The details of this approach are discussed in Appendix D. The bound state wave functions have the form:

\[
\varphi_m = \begin{cases}
    \varphi_{m1} & r < R_0, \\
    \varphi_{m2} & r \geq R_0,
\end{cases}
\]

(5.5)

where

\[
\varphi_{m1} = \sum_{\eta = \pm} N_{mJ1\eta} \begin{pmatrix}
    a_{mJ1\eta} I_{mJ-\frac{1}{2}}(k_{mJ1\eta} r) e^{i(mJ-\frac{1}{2})\theta} \\
    b_{mJ1\eta} I_{mJ+\frac{1}{2}}(k_{mJ1\eta} r) e^{i(mJ+\frac{1}{2})\theta} \\
    c_{mJ1\eta} I_{mJ+\frac{1}{2}}(k_{mJ1\eta} r) e^{i(mJ+\frac{1}{2})\theta} \\
    I_{mJ-\frac{1}{2}}(k_{mJ1\eta} r) e^{i(mJ-\frac{1}{2})\theta}
\end{pmatrix},
\]

(5.6)

and

\[
\varphi_{m2} = \sum_{\eta = \pm} N_{mJ2\eta} \begin{pmatrix}
    a_{mJ2\eta} e^{i(mJ-\frac{1}{2})\pi} K_{mJ-\frac{1}{2}}(k_{mJ2\eta} r) e^{i(mJ-\frac{1}{2})\theta} \\
    b_{mJ2\eta} e^{i(mJ+\frac{1}{2})\pi} K_{mJ+\frac{1}{2}}(k_{mJ2\eta} r) e^{i(mJ+\frac{1}{2})\theta} \\
    c_{mJ2\eta} e^{i(mJ+\frac{1}{2})\pi} K_{mJ+\frac{1}{2}}(k_{mJ2\eta} r) e^{i(mJ+\frac{1}{2})\theta} \\
    e^{i(mJ-\frac{1}{2})\pi} K_{mJ-\frac{1}{2}}(k_{mJ2\eta} r) e^{i(mJ-\frac{1}{2})\theta}
\end{pmatrix}.
\]

(5.7)
Figure 5.3. Spectrum of the in-gap dispersive states as a function of the total angular momentum quantum number $m_J$. Results are presented for two different sets of parameters: (a) $\mu_1 = 0.2$ meV, $\mu_2 = 0.4$ meV, $\Delta = 0.3$ meV, and (b) $\mu_1 = 0.1$ meV, $\mu_2 = 0.2$ meV, $\Delta = 0.2$ meV. We take $R_0 = 10$ nm and $\alpha = 0.25$ meV·nm.

The energy spectrum of these bound states vs the $m_J$ quantum numbers is presented in Fig. 5.3, while the spatial profile of the wave functions is given in Fig. 5.4 for two different characteristic sets of parameters. The number of in-gap states is quantized due to the finite
perimeter of the nanoflake and their energy spacing depends on the intrinsic parameters given in Eqs. (5.1) and (5.3). In the first set of parameters, we find 8 in-gap states while we have 4 in-gap states in the second set. We choose the strength of the Zeeman field such that the topological gap,

$$\Delta_{\text{top}} = \left| h - \sqrt{\Delta^2 + \mu^2} \right|,$$

(5.10)
is equal both inside and outside the nanoflake. We make this choice for simplicity, and note that our results do not qualitatively change for alternative choices of the Zeeman field strength as long as the quantity $\Delta_{\text{top}}(r) = h - \sqrt{\Delta^2 + \mu(r)^2}$ changes sign as $r = R_0$. From our first set of data we obtain $\Delta_{\text{top}} = 0.070$ meV, while for our second set we obtain $\Delta_{\text{top}} = 0.0296$ meV. The existence of only one branch of states in the topological gap signals that they are chiral (here left handed). This in turn supports the hypothesis of a phase separation in space with a chiral Majorana edge state circulating around the nanoflake.

We also note that these dispersive states are not perfectly linear, but instead exhibit a slight cubic behavior. Comparing both set of parameters, we see that the larger the discontinuity $|\delta \mu| = |\mu_1 - \mu_2|$, the more localized the edge states are. This behavior is expected; indeed, the in-gap Majorana states are pinned at the domain wall which is controlled by the spatial variation of the chemical potential.

5.3. Summary and Conclusions

Recent experimental results have presented the possibility of the emergence of non–trivial topological phases in magnetic nanostructures coupled to superconducting substrates [13, 76]. In this chapter, we have explored the artificial implementation of topological phase transitions induced by the local modification of the chemical potential. In this respect, we performed analytic calculations valid in the continuum limit in the case of a nanoflake with a circular geometry and found the spectrum of the system as a function of the total angular momentum. We have also studied how the transverse spatial extent of the wave function of the chiral Majorana state localized around the nanoflake depends upon the system parameters.
Figure 5.4. Localization of the in-gap bound states around the edge of the nanoflake for different values of the total angular momentum $m_J$. Figures (a) and (b) correspond to the same sets of parameter values as detailed in Fig. 5.3.
Chapter 6. Conclusion

In this dissertation we have studied the consequences of non-ideal material interfaces on Majorana bound states present at the boundaries of both topological insulators (TIs) and topological superconductors (TSCs). Focusing on TI-superconductor (SC) interfaces in Chapter 2, we assume the most general form of the Dirac Hamiltonian describing the TI interface state and obtain the proximity-induced superconducting order parameter of the TI-SC interface [7]. We show that for spin-singlet parent SCs, the magnitude of the proximity induced order parameter is the same as that of the parent. However, we find that the interface’s order parameter acquires a nontrivial complex phase as particles travel around the Brillouin zone, resulting topologically nontrivial superconductivity and under appropriate conditions allowing for the emergence of Majorana bound states [5]. For parent spin-triplet SCs on the other hand, the nature of the proximity-induced order parameter depends on the details of the TI-SC interface. One such example are chiral $p_x + ip_y$ SCs, which are only capable of inducing superconductivity onto the TI-SC boundary as long as the spin texture of the TI’s interface state contains components which point away from the interfacial plane. TI-vacuum surfaces are known to host helical surface states in which the the spins of the quasiparticles remain within the plane of the interface. However, out-of-plane spin textures are known to occur in TI interface states present in material junctions of TIs with other materials, and arise from interface potentials such as stress and shear strains [17]. This shows that interface potentials are critical in enabling the emergence of proximity-induced superconductivity in TI-SC heterostructures with parent spin-triplet SCs, which could lead to the presence of Majorana bound states within these systems [5].

To measure the consequences of these interface potentials, we adopt a specific model of the TI-interface state which we derived from the interface of a bulk three-dimensional TI crystal Hamiltonian with an included rotational symmetry breaking interface potential, allowing us to obtain a description of the out-of-plane spin component of the TI interface state as a function of the interface potential strength. We then calculate the experimentally measurable
signatures of the proximity-induced order parameter by focusing on chiral spin-triplet parent SCs and deriving the conductance spectra of lateral heterostructures, which comprise a TI crystal only half covered by a parent SC. Because the wave function matching between TI-vacuum and TI-SC interface states is nontrivial, we derive the proper boundary value relations between regions between two linear Hamiltonians by setting \( \psi_I = \mathcal{M} \psi_{II} \) (where \( \psi_I \) belongs to the TI-vacuum surface and \( \psi_{II} \) belongs to the TI-SC interface) and mandating that the total system Hamiltonian is Hermitian. We then obtain the conductance spectra of these structures for multiple types of rotational symmetry breaking interface potentials.

In Chapter 3 we elaborate on the details presented in Chapter 2 as we investigate both the normal state conductance and superconducting Andreev conductance signatures arising from nonhelical spin textures in lateral heterojunctions. We discuss the derivation of the boundary value matrix \( \mathcal{M} \) which results from the hermiticity of the total system Hamiltonian, and show how localized scattering at the one-dimensional boundary connecting the separate two-dimensional planes can lead to observable signatures in the normal state conductance spectra. Adopting these results to the case of superconducting lateral heterojunctions, we compare the consequences of scattering at the one-dimensional boundary to both mismatches of the chemical potential between the different regions, and to the effects of nonhelical spin textures arising from interface potentials within the TI-SC interface half of the heterojunction. We also analyze the difference in conductance signatures between systems with different types of interface potentials. Shear strains create an ellipticity in the interface states Fermi surface, and the direction of the strain determines the axes of ellipticity, leading to direction-dependent conductance signatures in the lateral heterostructure. Finally, we analyze the conductance spectra for several different symmetry families of parent spin-triplet SCs. For some helical SCs there is no proximity-induced superconductivity at all in the absence of rotational symmetry breaking interface potentials, similar to the chiral \( p_x + ip_y \) SCs studied in Chapter 2.
While many recent proposals for quantum computation rely on the use of zero-dimensional Majorana quasiparticles, which are difficult to energetically resolve against other low-energy states, in Chapter 4 we focus on recently observed one-dimensional chiral Majorana modes (CMMs) found on the boundaries of two-dimensional TSCs. In this chapter we demonstrate that smoothly varying band inversions generated by magnetic domain walls in both one-dimensional and two-dimensional SCs generate massive states known as Volkov-Pankratov (VP) states, in addition to the Majorana quasiparticles. We introduce a minimal model of an s-wave SC with Rashba spin-orbit coupling, and show that zero-energy Majorana excitations are accompanied by VP states whose energy gap is determined by the slope of the magnetic Zeeman exchange field associated with the domain wall. While the Majorana excitations are localized about the topological phase boundaries (TPBs), we show that the VP states are split in real space away from these boundaries. We also analyze how the Majorana and VP states are affected by in-plane electric fields. Despite being electrically neutral, their spatial positions may be controlled by the electric field strength. We also find that the energy level spacing of the VP states decreases as the electric field strength increases, which is a consequence of the relativistic effects of Lorentz boosts. We calculate the spin-resolved local density of states about the TPBs and find that the VP states are spatially spin-polarized with opposite spin polarizations on either side of the TPB, which we predict will be an observable signature through spin-resolved scanning tunneling spectroscopy experiments.

Finally, in Chapter 5 we analyze another avenue to obtain band inversions resulting in Majorana bound states. While Chapter 4 focused on systems with constant chemical potential and under a magnetic domain wall, here we instead analyze systems in which there is a spatially inhomogenous chemical potential held at a constant magnetic Zeeman energy. Specifically, we study the case in which a circular nanoflake composed of nonmagentic atoms in deposited on a two-dimensional SC, resulting in a localized region with an altered chemical potential. By taking advantage of the circular symmetry, we analytically derive the dispersive chiral Majorana bound states in terms of the total angular momentum quantum
numbers. We then calculate the spatial extent of these bound states in terms of the system parameters, and numerically determine their energy eigenvalues.

6.1. Ongoing Work and Future Projects

The important consequences of material interfaces addressed within this dissertation, along with the techniques used to discover them, have led to the creation of several new research directions. One such direction involves the use of CMMs to encode quantum information. While the above proposals for TIs and TSCs give rise to Majorana quasiparticles that could be used as topological qubits, none of them address how they are used to perform quantum computations. To encode quantum information, Majorana quasiparticles must be moved around one another. The TI proposal in Chapters 2 and 3 admit states sandwiched within a heterostructure with no obvious way to be controllably moved, and the TSC proposals in Chapters 4 and 5 are similarly fixed in their position.
A recent experimental setup capable of performing quantum computations is illustrated in Fig. 6.1 and is composed of a magnetically doped TI thin film in contact with a SC [62]. These TI thin films act differently than their bulk counterparts and form a class of materials known as quantum anomalous Hall insulators (QAHIs). Electrons are confined to travel around the one-dimensional edge of the thin film, and due to the magnetization, they must all travel in the same direction. At the same time, the SC hosts Majorana quasiparticle edge states like those discussed in Chapters 4 and 5. Applying a current through the device transforms the incoming electrons into TSC edge states, and quantum information is encoded as the motion is electrically controlled [64]. However, in Ref. [62] it is claimed that the observation of half-integer quantized conductance plateaus as the external magnetic field is swept give a distinct signature of Majorana fermion modes. These findings are currently under dispute, as recent theoretical and experimental work has found that these same experimental signatures can arise from a variety of nontopological sources [63, 65–67]. Our intention is to find how imperfections of the QAHI-SC material interface, such as those arising from interface potentials and VP states, affect the CMM’s ability to encode and store quantum information.

The application of topology in material science has led to many exciting developments for the construction of next-generation technologies. We hope that the proposals found within this dissertation offer a rich ground for future theoretical and experimental work.

“Stand at the base and look up at 3,000 feet of blankness. It just looks like there’s no way you can climb it. That’s what you seek as a climber. You want to find something that looks absurd and figure out how to do it.”

–Tommy Caldwell
Appendix A. Boundary Conditions for Dirac Hamiltonians

In this appendix we construct the boundary value matrix $\mathcal{M}(\beta)$ introduced in Chapters 2 and 3. This matrix is used to relate wave functions between planar regions described by different linear Dirac Hamiltonians. The free parameter $\beta$ quantifies the localized scattering at the one-dimensional boundary between the two planar regions. In Chapters 2 and 3, we use $\mathcal{M}(\beta)$ in the wave function matching as we calculate the conductance spectra of the lateral heterojunction, which comprise a topological insulator (TI) only half covered by a superconductor.

Consider two planar regions joined at $x = 0$ both described by linear Dirac Hamiltonians. We assume that the $x < 0$ half of space is a TI-vacuum surface, and may therefore be described by a helical surface Hamiltonian, while the $x > 0$ side is described by an arbitrary Dirac Hamiltonian \[7\]. However, even if this is not the case, we may always perform a coordinate transformation such that the $x < 0$ half of space has a circular Fermi surface, with the $x > 0$ half of space remaining arbitrary. Therefore, without loss of generality, we consider the system

$$H = \begin{cases} \hbar v_F (\sigma \times k)_z - \mu_L, & \text{as } x < 0 \\ \sigma \cdot c(k) - \mu_R, & \text{as } x > 0 \end{cases} \tag{A.1}$$

Here $c_i(k) = \sum_j c_{ij}k_j$. From Ref. [102], we have that $\hbar v_F = A_2$, so we can rewrite

$$H = \begin{cases} A_2(\sigma_xk_y - \sigma_yk_x) - \mu_L, & \text{as } x < 0 \\ c_{xx}k_x + c_{xy}\sigma_xk_y + c_{yx}\sigma_yk_x + c_{yy}\sigma_yk_y + c_{zz}\sigma_zk_z + c_{zy}\sigma_yk_y - \mu_R, & \text{as } x > 0 \end{cases} \tag{A.2}$$

Because translational symmetry is broken along the $\hat{x}$-direction, we must replace $k_x \rightarrow -i\partial_x$.

For the total Hamiltonian $H$ to obey hermiticity, we must have that

$$\langle \psi_1 | H \psi_2 \rangle = \langle H \psi_1 | \psi_2 \rangle \tag{A.3}$$
Here we define the inner product as an integral over $x$. Let us write

$$H = \Theta(-x)H_L + \Theta(x)H_R$$  \hspace{1cm} (A.4)

$$\psi(x) = \Theta(-x)\psi_L(x) + \Theta(x)\psi_R(x)$$  \hspace{1cm} (A.5)

Here we keep in mind that $\psi_L(x)$ and $\psi_R(x)$ are spinors. Focusing on the left term of the hermiticity equation, we have that

$$\langle \psi_1 | H | \psi_2 \rangle = \int_{-\infty}^{0} \psi_{1L}^\dagger(x)H_L\psi_{2L}(x)dx + \int_{0}^{\infty} \psi_{1R}^\dagger(x)H_R\psi_{2R}(x)dx$$  \hspace{1cm} (A.6)

$$= \int_{-\infty}^{0} \psi_{1L}^\dagger \left[ A_2\sigma_xk_y - A_2\sigma_y(-i\partial_x) - \mu_L \right] \psi_{2L} dx$$

$$+ \int_{0}^{\infty} \psi_{1R}^\dagger \left[ c_{xx}\sigma_x(-i\partial_x) + c_{xy}\sigma_zk_y + c_{yx}\sigma_y(-i\partial_x) + c_{yy}\sigma_yk_y + c_{zx}\sigma_z(-i\partial_x) - \mu_R \right] \psi_{2R} dx$$

$$= \int_{-\infty}^{0} \psi_{1L}^\dagger \left[ -A_2\sigma_y(-i\partial_x) \right] \psi_{2L} dx$$

$$+ \int_{0}^{\infty} \psi_{1R}^\dagger \left[ c_{xx}\sigma_x(-i\partial_x) + c_{xy}\sigma_y(-i\partial_x) + c_{zx}\sigma_z(-i\partial_x) \right] \psi_{2R} dx$$

$$+ \int_{-\infty}^{0} \psi_{1L}^\dagger \left[ A_2\sigma_zk_y - \mu_L \right] \psi_{2L} dx$$

$$+ \int_{0}^{\infty} \psi_{1R}^\dagger \left[ c_{xy}\sigma_zk_y + c_{yy}\sigma_yk_y + c_{zy}\sigma_zk_y - \mu_R \right] \psi_{2R} dx$$
Integrating by parts, we find that

\[
\langle \psi_1 | H \psi_2 \rangle = \left( \psi_{1L}^\dagger \left[ -A_2 \sigma_y(-i) \right] \psi_{2L} \right)_0^0 - \int_{-\infty}^0 (\partial_x \psi_{1L}^\dagger) \left[ -A_2 \sigma_y(-i) \right] \psi_{2L} \, dx
\]

\[
+ \left( \psi_{1R}^\dagger \left[ c_{xx} \sigma_x(-i) + c_{yy} \sigma_y(-i) + c_{xz} \sigma_z(-i) \right] \psi_{2R} \right)_0^0 \]

\[
- \int_0^\infty (\partial_x \psi_{1R}^\dagger) \left[ c_{xx} \sigma_x(-i) + c_{yy} \sigma_y(-i) + c_{xz} \sigma_z(-i) \right] \psi_{2R} \, dx
\]

\[
+ \int_{-\infty}^0 \psi_{1R}^\dagger \left[ A_2 \sigma_x k_y - \mu_L \right] \psi_{2L} \, dx
\]

\[
+ \int_0^\infty \psi_{1L}^\dagger \left[ c_{xy} \sigma_x k_y + c_{yy} \sigma_y k_y + c_{zy} \sigma_z k_y - \mu_L \right] \psi_{2R} \, dx
\]

Now, note that

\[
\langle \psi_2 | H \psi_1 \rangle = \int_{-\infty}^0 \psi_{2L}^\dagger \left[ A_2 \sigma_x k_y - A_2 \sigma_y(-i \partial_x) - \mu_L \right] \psi_{1L} \, dx
\]

\[
+ \int_{0}^\infty \psi_{2R}^\dagger \left[ c_{xx} \sigma_x(-i \partial_x) + c_{xy} \sigma_x k_y + c_{yy} \sigma_y(-i \partial_x) + c_{yy} \sigma_y k_y + c_{zy} \sigma_z k_y - \mu_L \right] \psi_{1R} \, dx
\]

\[
\langle H \psi_1 | \psi_2 \rangle = \langle \psi_2 | H \psi_1 \rangle^* = \frac{\langle \psi_2 | \psi_2 \rangle}{\langle \psi_2 | \psi_2 \rangle}
\]

\[
= \int_{-\infty}^0 \psi_{1L}^\dagger \left[ A_2 \sigma_x k_y \right] \psi_{2L} \, dx + \int_{-\infty}^0 (\partial_x \psi_{1L}^\dagger) \left[ -A_2 \sigma_y(i) \right] \psi_{2L} \, dx - \int_{-\infty}^0 \psi_{1L}^\dagger \mu_L \psi_{2L} \, dx
\]

\[
+ \int_{0}^\infty \psi_{1R}^\dagger \left[ c_{xy} \sigma_x k_y + c_{yy} \sigma_y k_y + c_{zy} \sigma_z k_y \right] \psi_{2R} \, dx
\]

\[
+ \int_{0}^\infty (\partial_x \psi_{1R}^\dagger) \left[ c_{xx} \sigma_x(i) + c_{yx} \sigma_y(i) + c_{zy} \sigma_z(i) \right] \psi_{2R} \, dx - \int_{0}^\infty \psi_{1R}^\dagger \mu_R \psi_{2R} \, dx
\]

In the above we have used the relation \( \langle \phi | A | \psi \rangle^* = \langle \psi | A^\dagger | \phi \rangle \) for the spinors and the Pauli matrices within the integrals. Thus, we can observe that

\[
\langle \psi_1 | H \psi_2 \rangle = \left( \psi_{1L}^\dagger \left[ -A_2 \sigma_y(-i) \right] \psi_{2L} \right)_0^0
\]

\[
+ \left( \psi_{1R}^\dagger \left[ c_{xx} \sigma_x(-i) + c_{yy} \sigma_y(-i) + c_{xz} \sigma_z(-i) \right] \psi_{2R} \right)_0^0
\]

\[
+ \langle H \psi_1 | \psi_2 \rangle
\]

\[
(A.10)
\]
The requirement of hermiticity can then be expressed as

\[
\left(\psi_{1L}^\dagger \left[ -A_2 \sigma_y(-i) \right] \psi_{2L} \right)_0^0 + \left(\psi_{1R}^\dagger \left[ c_{xx} \sigma_x(-i) + c_{yz} \sigma_y(-i) + c_{zx} \sigma_z(-i) \right] \psi_{2R} \right)_0^\infty = 0 \quad (A.11)
\]

Let us assume that the wave functions are “well behaved” at infinity, and go to zero as \(x \to \pm \infty\). The above statement then becomes

\[
\psi_{1L}^\dagger(0) \left[ -A_2 \sigma_y(-i) \right] \psi_{2L}(0) = \psi_{1R}^\dagger(0) \left[ c_{xx} \sigma_x(-i) + c_{yz} \sigma_y(-i) + c_{zx} \sigma_z(-i) \right] \psi_{2R}(0) \quad (A.12)
\]

Now, at the boundary, let us assume

\[
\psi_L(0) = M \psi_R(0) \quad (A.13)
\]

Here \(M\) is an arbitrary matrix,

\[
M = \sum \alpha_i \sigma_i \quad (A.14)
\]

\[
= \alpha_0 \sigma_0 + \alpha_x \sigma_x + \alpha_y \sigma_y + \alpha_z \sigma_z
\]

Here \(\alpha_i \in \mathbb{C}\). We are then lead to the condition

\[
M^\dagger \left[ -A_2 \sigma_y \right] M = c_{xx} \sigma_x + c_{yz} \sigma_y + c_{zx} \sigma_z \quad (A.15)
\]

We shall quickly demonstrate that, if \(M\) commutes with the time reversal operator \(T = i \sigma_y K\), then the spinors \(\psi_L(0)\) and \(\psi_R(0)\) shall preserve Kramers degeneracy. Here \(K\) is the complex conjugation operator. First, we shall find the conditions on the \(\alpha_i\) coefficients such
that \([M, T] = 0\). We see that

\[
[M, T] = MT - TM \tag{A.16}
\]

\[
= \left[\alpha_0\sigma_0 + \alpha_x\sigma_x + \alpha_y\sigma_y + \alpha_z\sigma_z\right] (i\sigma_y K) - (i\sigma_y K) \left[\alpha_0\sigma_0 + \alpha_x\sigma_x + \alpha_y\sigma_y + \alpha_z\sigma_z\right]
\]

\[
= \left[\alpha_0\sigma_0 + \alpha_x\sigma_x + \alpha_y\sigma_y + \alpha_z\sigma_z\right] (i\sigma_y K) - (i\sigma_y K) \left[\alpha_0^*\sigma_0^* + \alpha_x^*\sigma_x^* - \alpha_y^*\sigma_y^* + \alpha_z^*\sigma_z^*\right] (K)
\]

\[
= \left[\alpha_0\sigma_0 + i\alpha_x\sigma_x + \alpha_y\sigma_0 - i\alpha_z\sigma_z\right] (iK) - \left[\alpha_0^*\sigma_0^* - i\alpha_x^*\sigma_x^* - \alpha_y^*\sigma_y^* + i\alpha_z^*\sigma_z^*\right] (iK)
\]

\[
= 0
\]

Thus we have that

\[
\alpha_0\sigma_0 + i\alpha_x\sigma_x + \alpha_y\sigma_0 - i\alpha_z\sigma_z = \alpha_0^*\sigma_0^* - i\alpha_x^*\sigma_x^* - \alpha_y^*\sigma_y^* + i\alpha_z^*\sigma_z^* \tag{A.17}
\]

This implies

\[
\alpha_0 = \alpha_0^* \tag{A.18}
\]

\[
\alpha_x = -\alpha_x^*
\]

\[
\alpha_y = -\alpha_y^*
\]

\[
\alpha_z = -\alpha_z^*
\]

This means that \(\alpha_0 \in \mathbb{R}\), and \(\alpha_x, \alpha_y, \alpha_z \in \mathbb{I}\). Letting \(\gamma_i\) be real, we can write

\[
M = \gamma_0\sigma_0 + i(\gamma_x\sigma_x + \gamma_y\sigma_y + \gamma_z\sigma_z) \tag{A.19}
\]
It can quickly be shown that \( M^\dagger M = \sum_i \gamma_i^2 \sigma_0 \). We can then show that Kramers degeneracy is preserved at the interface, as

\[
\psi_L^\dagger(0) T \psi_L(0) = \psi_R^\dagger(0) M^\dagger T M \psi_R(0) = \psi_R^\dagger(0) M^\dagger M T \psi_R(0) = \sum_i \gamma_i^2 \psi_R^\dagger(0) T \psi_R(0)
\]

Thus, if \( \psi_R^\dagger(0) T \psi_R(0) = 0 \), then \( \psi_L^\dagger(0) T \psi_L(0) = 0 \).

Now, in terms of the \( \gamma_i \) coefficients, the condition for \( M \) becomes

\[
(\gamma_0 \sigma_0 - i\gamma_x \sigma_x - i\gamma_y \sigma_y - i\gamma_z \sigma_z) \left[ -A_2 \sigma_y \right] (\gamma_0 \sigma_0 + i\gamma_x \sigma_x + i\gamma_y \sigma_y + i\gamma_z \sigma_z)
\]

\[
= c_{xx} \sigma_x + c_{yx} \sigma_y + c_{xz} \sigma_z
\]

Solving in Mathematica gives, using the Einstein summation convention,

\[
\gamma_0 = \pm \sqrt{-c_{yx} + \sqrt{c_{ix} c_{ix}}} - \gamma_y^2
\]

\[
\gamma_x = -\frac{c_{yx} + \sqrt{c_{ix} c_{ix}}}{c_{xx}^2 + c_{zz}^2} \left( c_{xx} \gamma_y \pm c_{xx} \sqrt{-\frac{c_{yx} + \sqrt{c_{ix} c_{ix}}}{2A_2} - \gamma_y^2} \right)
\]

\[
\gamma_y = \gamma_y
\]

\[
\gamma_z = \frac{c_{yz} + \sqrt{c_{ix} c_{ix}}}{c_{xx}^2 + c_{zz}^2} \left( \pm c_{xx} \sqrt{-\frac{c_{yx} + \sqrt{c_{ix} c_{ix}}}{2A_2} - \gamma_y^2 - c_{xx} \gamma_y} \right)
\]

Here the summation goes over \( i = x, y, z \). We see that \( \gamma_y \) is a free parameter. But, in order for all the \( \gamma_i \) to be real, we must have that

\[
-\sqrt{-\frac{c_{yx} + \sqrt{c_{ix} c_{ix}}}{2A_2}} < \gamma_y < \sqrt{-\frac{c_{yx} + \sqrt{c_{ix} c_{ix}}}{2A_2}}
\]
Let us write

$$\gamma_y = \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}} \frac{\sin \beta}{2A_2}$$  \hspace{1cm} (A.24)$$

This then gives us

$$\gamma_0 = \pm \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}} \frac{\cos \beta}{2A_2}$$  \hspace{1cm} (A.25)$$

$$\gamma_x = -\frac{c_{xx} \sin \beta \pm c_{zx} \cos \beta}{\sqrt{2A_2} \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}}}$$

$$\gamma_y = \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}} \frac{\sin \beta}{2A_2}$$

$$\gamma_z = \pm \frac{c_{xx} \cos \beta - c_{zx} \sin \beta}{\sqrt{2A_2} \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}}}$$

We can then choose $\pm |\cos \beta| \rightarrow \cos \beta$ for our problem.

For the case of holes, we must switch $\sigma_y \rightarrow -\sigma_y$ in our starting Hamiltonians $H_L$ and $H_R$, as well as $\mu_{L,R} \rightarrow -\mu_{L,R}$. This is because the hole Hamiltonians are given by $-H^T(-k)$. Solving the boundary value matrix condition for holes, $\mathcal{M}_h$, we obtain

$$\gamma_{0h} = \pm \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}} \frac{\cos \beta}{2A_2}$$  \hspace{1cm} (A.26)$$

$$\gamma_{xh} = \frac{c_{xx} \sin \beta \pm c_{zx} \cos \beta}{\sqrt{2A_2} \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}}}$$

$$\gamma_{yh} = \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}} \frac{\sin \beta}{2A_2}$$

$$\gamma_{zh} = -\frac{c_{xx} \cos \beta - c_{zx} \sin \beta}{\sqrt{2A_2} \sqrt{-c_{yx} + \sqrt{c_{ix}c_{ix}}}}$$

Again we choose $\pm |\cos \beta| \rightarrow \cos \beta$. The boundary value matrix which connects the left and right wave functions of our Andreev reflection problem is then given by

$$\mathcal{M}_{BDG} = \begin{pmatrix} \mathcal{M} & 0 \\ 0 & \mathcal{M}_h \end{pmatrix}$$  \hspace{1cm} (A.27)$$
Appendix B. Hyperbolic Tangent Magnetic Field Profiles in Two-Dimensional Superconductors

In this appendix we analyze a two-dimensional superconductor (SC) with large Rashba spin-orbit coupling under a magnetic domain wall, such that the profile of the magnetic Zeeman exchange field is described by a hyperbolic tangent function. In Chapter 4, we modeled magnetic domain walls on one-dimensional and two-dimensional SCs by assuming a linear Zeeman exchange field profile, as given in Eq. (4.5). We shall demonstrate that if we instead assume a tanh-like exchange field profile, we will obtain the same qualitative spectra as shown in Fig. 4.6 given by the linear case.

Focusing on small momenta, the first quantized real-space Hamiltonian describing our two-dimensional SC with Rashba spin-orbit coupling, in the absence of superconductivity, is given by

$$H(r, \nabla) = \alpha(\sigma \times -i\nabla)_z + B(y)\sigma_z$$  \hspace{1cm} (B.1)

Here the system is two dimensional with $r = (x, y)$. The Zeeman exchange field is given by

$$B(y) = \Delta[1 + \tanh(y/\ell)].$$  \hspace{1cm} (B.2)

Here $\ell$ determines the width of the interface. In Fig. B.1 we plot this exchange field profile in the case that $\ell > \alpha/\Delta$, which constitutes a smooth interface. The second quantized real-space BdG Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2} \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \begin{pmatrix} H(\mathbf{r}, \nabla) & i\sigma_y \Delta \\ -i\sigma_y \Delta & -H^T(\mathbf{r}, -\nabla) \end{pmatrix} \Psi(\mathbf{r})$$  \hspace{1cm} (B.3)

Here $\Psi(\mathbf{r}) = (\psi^\uparrow(\mathbf{r}), \psi^\downarrow(\mathbf{r}), \psi^\uparrow_\dagger(\mathbf{r}), \psi^\downarrow_\dagger(\mathbf{r}))^T$, where $\psi_\sigma(\mathbf{r})$ are electron field operators which destroy an electron at location $\mathbf{r}$. Let us write

$$\psi_\sigma(\mathbf{r}) = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \psi_{k\sigma}(y).$$  \hspace{1cm} (B.4)
Figure B.1. Magnetic Zeeman exchange field profile with a characteristic interface width given by $\ell$. Here $\ell > \alpha/\Delta$, which creates a smooth interface.

Here $k$ is the momentum along the topological phase boundary, and $L$ is the length of the one-dimensional topological phase boundary. Inserting this into the Hamiltonian gives

$$
\mathcal{H} = \frac{1}{2} \sum_k \int dy \Psi_k^\dagger(y) \begin{pmatrix}
B(y) & \alpha(-i\partial_y + ik) & 0 & \Delta \\
\alpha(-i\partial_y - ik) & -B(y) & -\Delta & 0 \\
0 & -\Delta & -B(y) & \alpha(-i\partial_y - ik) \\
\Delta & 0 & \alpha(-i\partial_y + ik) & B(y)
\end{pmatrix} \Psi_k(y)
$$

(B.5)

Here we have

$$
\Psi_k(y) = (\psi_{k\uparrow}(y), \psi_{k\downarrow}(y), \psi_{-k\uparrow}(y), \psi_{-k\downarrow}(y))^T
$$

(B.6)
To simplify the matrix Hamiltonian we introduce the unitary matrix
\[
U = \frac{e^{-i\pi/4}}{2} \begin{pmatrix}
-1 & 1 & -1 & 1 \\
-i & i & i & -i \\
i & i & -i & -i \\
1 & 1 & 1 & 1
\end{pmatrix}.
\]  
(B.7)

This allows us to write
\[
\mathcal{H} = \frac{1}{2} \sum_k \int dy [U^\dagger \Psi_k(y)]^\dagger \times \begin{pmatrix}
-\alpha k & 0 & B(y) - \Delta - \alpha \partial_y & 0 \\
0 & -\alpha k & 0 & B(y) + \Delta - \alpha \partial_y \\
B(y) - \Delta + \alpha \partial_y & 0 & \alpha k & 0 \\
0 & B(y) + \Delta + \alpha \partial_y & 0 & \alpha k
\end{pmatrix} \times [U^\dagger \Psi_k(y)]
\]  
(B.8)

Let us define
\[
\hat{a}_\pm = B(y) \pm \Delta + \alpha \partial_y
\]  
(B.9)

We then wish to find the eigenvalues of the $4 \times 4$ matrix Hamiltonian such that
\[
\begin{pmatrix}
-\alpha k & 0 & \hat{a}_-^\dagger & 0 \\
0 & -\alpha k & 0 & \hat{a}_+^\dagger \\
\hat{a}_- & 0 & \alpha k & 0 \\
0 & \hat{a}_+ & 0 & \alpha k
\end{pmatrix} \varphi = E \varphi
\]  
(B.10)
Squaring the Hamiltonian gives

\[
\begin{pmatrix}
\hat{a}_-\hat{a}_+ - (E^2 - \alpha^2 k^2) & 0 & 0 & 0 \\
0 & \hat{a}_\dagger_- \hat{a}_+ - (E^2 - \alpha^2 k^2) & 0 & 0 \\
0 & 0 & \hat{a}_-\hat{a}_\dagger_+ - (E^2 - \alpha^2 k^2) & 0 \\
0 & 0 & 0 & \hat{a}_\dagger_- \hat{a}_\dagger_+ - (E^2 - \alpha^2 k^2)
\end{pmatrix} \times \varphi = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.
\] (B.11)

Consider \(\varphi = (\phi_+, 0, \phi_-, 0)^T\) and \(\tilde{\varphi} = (0, \tilde{\phi}_+, 0, \tilde{\phi}_-)^T\). The above system of equations then has the form

\[
\begin{pmatrix}
\frac{1}{2} \left\{ \hat{a}_\dagger_- \hat{a}_+ \pm [\hat{a}_\dagger_-, \hat{a}_+] \right\} - (E^2 - \alpha^2 k^2) \\
\frac{1}{2} \left\{ \hat{a}_\dagger_+ \hat{a}_+ \pm [\hat{a}_\dagger_+, \hat{a}_+] \right\} - (E^2 - \alpha^2 k^2)
\end{pmatrix} \varphi_{\pm} = 0,
\] (B.12)

From here we shall focus on the first set of equations that include the \(\hat{a}_-\) operators. The second set of equations including \(\hat{a}_+\) do not correspond to bound states with energies below the superconducting gap.

From the definition of \(B(y)\) we have that

\[
\hat{a}_- = B(y) - \Delta + \alpha \partial_y \\
= \operatorname{tanh}(y/\ell) \Delta + \alpha \partial_y
\] (B.13)

Consider the following change of variables

\[
s = \frac{1}{2} [1 - \operatorname{tanh}(y/\ell)]
\] (B.14)
From \( \frac{d}{dy} = \frac{ds}{dy} \frac{d}{ds} \), we find

\[
\frac{ds}{dy} = \frac{d}{dy} \left[ \frac{1}{2} - \frac{1}{2} \tanh(y/\ell) \right] \]

\[
= -\frac{1}{2} [1 - \tanh^2(y/\ell)] \frac{1}{\ell}
\]

Note that \( 1 - s = \frac{1}{2} + \frac{1}{2} \tanh(y/\ell) \), and that \( s(1 - s) = \frac{1}{4} [1 - \tanh^2(y/\ell)] \). Thus

\[
\frac{ds}{dy} = -2s(1 - s) \frac{1}{\ell}
\]

\[
\frac{d}{dy} = -\frac{2}{\ell} s(1 - s) \frac{d}{ds}
\]

Also, we see that

\[
s = \frac{1}{2} - \frac{1}{2} \tanh(y/\ell)
\]

\[-2s + 1 = \tanh(y/\ell)\]

\[\Delta(1 - 2s) = \Delta \tanh(y/\ell)\]

This all gives

\[
\dot{a}_- = \tanh(y/\ell) \Delta + \alpha \partial_y
\]

\[
= -\frac{2\alpha}{\ell} s(1 - s) \partial_s + \Delta - 2\Delta s
\]

We also have that

\[
\dot{a}^- = \frac{2\alpha}{\ell} s(1 - s) \partial_s + \Delta - 2\Delta s
\]
Let us then find $\hat{a}_+^\dagger \hat{a}_-$ and $\hat{a}_- \hat{a}_+^\dagger$. First, letting $f(s)$ be a test function, we have

$$\hat{a}_+^\dagger \hat{a}_- f(s) = \left[ \frac{2\alpha}{\ell} s(1-s) \partial_s + \Delta - 2\Delta s \right] \left[ - \frac{2\alpha}{\ell} s(1-s) \partial_s + \Delta - 2\Delta s \right] f(s) \quad (B.20)$$

$$= \left[ \frac{2\alpha}{\ell} s(1-s) \partial_s + \Delta - 2\Delta s \right] \left[ - \frac{2\alpha}{\ell} s(1-s) \frac{df}{ds} + \Delta f(x) - 2\Delta s f(s) \right]$$

$$= \frac{2\alpha}{\ell} s(1-s) \left( - \frac{2\alpha}{\ell} \right) \left\{ (1-s) \frac{df}{ds} - s \frac{df}{ds} + s(1-s) \frac{df^2}{ds^2} \right\}$$

$$+ \frac{2\alpha}{\ell} s(1-s) \Delta \frac{df}{ds} + \frac{2\alpha}{\ell} s(1-s)(-2\Delta) \left\{ f(s) + \frac{df}{ds} \right\}$$

$$+ (\Delta - 2\Delta s) \left[ - \frac{2\alpha}{\ell} s(1-s) \frac{df}{ds} + \Delta f(s) - 2\Delta s f(s) \right]$$

$$= - \left( \frac{2\alpha}{\ell} \right)^2 s^2 (1-s)^2 \frac{d^2 f}{ds^2} - \left( \frac{2\alpha}{\ell} \right)^2 s(1-s)(1-2s) \frac{df}{ds}$$

$$+ \frac{2\alpha}{\ell} s(1-s)(-2\Delta) f(s) + (\Delta - 2\Delta s)(\Delta - 2\Delta s) f(s)$$

$$= \left[ - \left( \frac{2\alpha}{\ell} \right)^2 s^2 (1-s)^2 \partial_s^2 \right.$$  

$$- \left( \frac{2\alpha}{\ell} \right)^2 s(1-s)(1-2s) \partial_s + \Delta^2 (1-2s)^2 - \frac{4\alpha \Delta}{\ell} s(1-s) \right] f(s)$$

This gives

$$[\hat{a}_+^\dagger \hat{a}_- - (E^2 - \alpha^2 k^2)] \phi_+ = 0 \quad (B.21)$$

$$\left[ - \left( \frac{2\alpha}{\ell} \right)^2 s^2 (1-s)^2 \partial_s^2 \right.$$  

$$- \left( \frac{2\alpha}{\ell} \right)^2 s(1-s)(1-2s) \partial_s + \Delta^2 (1-2s)^2 - (E^2 - \alpha^2 k^2) - \frac{4\alpha \Delta}{\ell} s(1-s) \right] \phi_+ = 0$$

$$\left[ s(1-s) \partial_s^2 + (1-2s) \partial_s - \left( \frac{\ell}{2\alpha} \right)^2 \left\{ \frac{\Delta^2 (1-2s)^2 - (E^2 - \alpha^2 k^2)}{s(1-s)} - \frac{4\alpha \Delta}{\ell} \right\} \right] \phi_+ = 0$$
For \( \hat{a}_-\hat{a}_+ \), we then have

\[
\hat{a}_-\hat{a}_+ f(s) = \left[ -\frac{2\alpha}{\ell} s(1-s)\partial_s + \Delta - 2\Delta s \right] \left[ \frac{2\alpha}{\ell} s(1-s)\partial_s + \Delta - 2\Delta s \right] f(s) \quad (B.22)
\]

\[
= \left[ -\frac{2\alpha}{\ell} s(1-s)\partial_s + \Delta - 2\Delta s \right] \left[ \frac{2\alpha}{\ell} s(1-s) \frac{df}{ds} + \Delta f(x) - 2\Delta s f(s) \right]
\]

\[
= -\frac{2\alpha}{\ell} s(1-s) \left( \frac{2\alpha}{\ell} \right) \left\{ (1-s) \frac{df}{ds} - s \frac{df}{ds} + s(1-s) \frac{df}{ds^2} \right\}
\]

\[
- \frac{2\alpha}{\ell} s(1-s)\Delta \frac{df}{ds} - \frac{2\alpha}{\ell} s(1-s)(-2\Delta) \left\{ f(s) + s \frac{df}{ds} \right\}
\]

\[
+ (\Delta - 2\Delta s) \left[ \frac{2\alpha}{\ell} s(1-s) \frac{df}{ds} + \Delta f(s) - 2\Delta s f(s) \right]
\]

\[
= -\left( \frac{2\alpha}{\ell} \right)^2 s^2(1-s)^2 \frac{d^2 f}{ds^2} - \left( \frac{2\alpha}{\ell} \right)^2 s(1-s)(1-2s) \frac{df}{ds}
\]

\[
+ \frac{2\alpha}{\ell} s(1-s)(2\Delta)f(s) + (\Delta - 2\Delta s)(\Delta - 2\Delta s)f(s)
\]

\[
= \left[ -\left( \frac{2\alpha}{\ell} \right)^2 s^2(1-s)^2 \partial_s^2
\right.
\]

\[
- \left( \frac{2\alpha}{\ell} \right)^2 s(1-s)(1-2s)\partial_s + \Delta^2(1-2s)^2 + \frac{4\alpha\Delta}{\ell} s(1-s) \right] f(s)
\]

This gives

\[
[\hat{a}_-\hat{a}_+ - (E^2 - \alpha^2k^2)]\phi_- = 0 \quad (B.23)
\]

\[
\left[ -\left( \frac{2\alpha}{\ell} \right)^2 s^2(1-s)^2 \partial_s^2
\right.
\]

\[
- \left( \frac{2\alpha}{\ell} \right)^2 s(1-s)(1-2s)\partial_s + \Delta^2(1-2s)^2 - (E^2 - \alpha^2k^2) + \frac{4\alpha\Delta}{\ell} s(1-s) \right] \phi_- = 0
\]

\[
\left[ s(1-s)\partial_s^2 + (1-2s)\partial_s - \left( \frac{\ell}{2\alpha} \right)^2 \left\{ \frac{\Delta^2(1-2s)^2 - (E^2 - \alpha^2k^2)}{s(1-s)} + \frac{4\alpha\Delta}{\ell} \right\} \right] \phi_- = 0
\]

Let \( \sigma = \pm \). We then have

\[
\left[ s(1-s)\partial_s^2 + (1-2s)\partial_s - \left( \frac{\ell}{2\alpha} \right)^2 \left\{ \frac{\Delta^2(1-2s)^2 - (E^2 - \alpha^2k^2)}{s(1-s)} - \sigma \frac{4\alpha\Delta}{\ell} \right\} \right] \phi_\sigma = 0 \quad (B.24)
\]
Replacing the wave function by $\phi_\sigma(s) = s^\alpha(1-s)^\beta u_\sigma(s)$ to remove the singularities, we obtain Euler’s hypergeometric equation. This exact equation was studied in detail in the supplementary material of Tchoumakov et al.’s 2017 publication [84]. The eigenenergies have been found to have the form

$$E = \pm \sqrt{\alpha^2k^2 - \frac{1}{4}[g_\sigma^2(n) - 4\Delta^2]}.$$  \hspace{1cm} (B.25)

Here the quantization is given by

$$g_\sigma(n) = \left| \frac{2\alpha}{\ell} \left[ \frac{1}{2} + \sigma \frac{\ell\Delta}{\alpha} \right] - \left(n + \frac{1}{2}\right) \right|.$$ \hspace{1cm} (B.26)

Here $n \in \mathbb{N}$. However, in this case, $n$ does not go up to infinity. Instead, $n$ starts at zero, and only goes up to the largest integer such that

$$g_\sigma(n) > 0.$$ \hspace{1cm} (B.27)

The dispersion of the low-energy bound states localized at $y = 0$ is given in Fig. B.2. We find that as $\ell$ becomes shorter, the additional massive states go above the superconducting gap. As $\ell$ increases, more massive states enter below the superconducting gap. We note that because we explicitly solved the square of the Hamiltonian, we have not mathematically determined the chirality of the $n = 0$ Majorana state, given by the red dotted line. (That is, the sign of the slope of the red dotted line). However, from our knowledge of the system and our previous work, we can infer that the $n = 0$ energy is given by $E = -\alpha k$. 

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Figure B.2. The dispersion of the low-energy bound states localized at $y = 0$, under the presence of a magnetic exchange field as given by Fig. B.1.
Appendix C. Hyperbolic Transformations on Dirac Hamiltonians

In this appendix we analyze a two-dimensional superconductor with large Rashba spin-orbit coupling under a linearly varying magnetic Zeeman exchange field and an in-plane electric field. In Chapter 4, we modeled the effects of the in-plane electric field through a linearly varying chemical potential, and simplified the system’s Bogoliubov-de Gennes (BdG) Hamiltonian by applying the hyperbolic transformation given in Eq. (4.17). Below we analyze the consequences hyperbolic transformations have on matrix Hamiltonians. We study the effects these transformations have on both a generic $2 \times 2$ matrix Hamiltonian, and on the $4 \times 4$ matrix Hamiltonian given in Eq. (4.17).

C.1. Hyperbolic Transformations on $2 \times 2$ Hamiltonians

We first analyze some properties of the operator $e^{\eta \sigma_b/2}$. Letting $a, b \in \{x, y, z\}$, we see that

\begin{equation}
 e^{\eta \sigma_b/2} \sigma_a e^{\eta \sigma_b/2} = e^{\eta \sigma_b/2} \sigma_a [\cosh(\eta/2)\sigma_0 + \sinh(\eta/2)\sigma_b] \tag{C.1}
\end{equation}

\[= [\cosh(\eta/2)\sigma_0 + \sinh(\eta/2)\sigma_b] [\cosh(\eta/2)\sigma_a + \sinh(\eta/2)(\delta_{ab}\sigma_0 + i\epsilon_{abi}\sigma_i)] \]

\[= \cosh^2(\eta/2)\sigma_a + \cosh(\eta/2)\sinh(\eta/2)(\delta_{ab}\sigma_0 + i\epsilon_{abi}\sigma_i) + \cosh(\eta/2)\sinh(\eta/2)(\delta_{ba}\sigma_0 + i\epsilon_{bai}\sigma_i) + \sinh^2(\eta/2)(\delta_{ab}\sigma_0 + i\epsilon_{abi}\sigma_i) \]

\[= \cosh^2(\eta/2)\sigma_a + \cosh(\eta/2)\sinh(\eta/2)(\delta_{ab}\sigma_0 + i\epsilon_{abi}\sigma_i) + \sinh^2(\eta/2)(\delta_{ab}\sigma_0 - (1 - \delta_{ab})\sigma_a) \]

\[= \cosh^2(\eta/2)\sigma_a + 2\cosh(\eta/2)\sinh(\eta/2)\delta_{ab}\sigma_0 + \sinh^2(\eta/2)(2\delta_{ab}\sigma_a - \sigma_a) \]

\[= [\cosh^2(\eta/2) - (2\delta_{ab} - 1)\sinh^2(\eta/2)]\sigma_a + \sinh(\eta)\delta_{ab}\sigma_0 \]

If $a = b$, we have

\begin{equation}
 e^{\eta \sigma_b/2} \sigma_b e^{\eta \sigma_b/2} = \cosh(\eta)\sigma_b + \sinh(\eta)\sigma_0 \tag{C.2}
\end{equation}

If $a \neq b$, we have

\begin{equation}
 e^{\eta \sigma_b/2} \sigma_a e^{\eta \sigma_b/2} = \sigma_a \tag{C.3}
\end{equation}
If $\sigma_a \rightarrow \sigma_0$, we have

$$e^{-\eta \sigma_z/2} \sigma_0 e^{\eta \sigma_z/2} = \cosh(\eta)\sigma_0 + \sinh(\eta)\sigma_b$$  \hspace{1cm} (C.4)

With these relations in hand, let us analyze the generic $2 \times 2$ Hamiltonian

$$H = h_0 + \mathbf{h} \cdot \mathbf{\sigma}$$  \hspace{1cm} (C.5)

$$= h_0\sigma_0 + h_x\sigma_x + h_y\sigma_y + h_z\sigma_z$$

Generically, we have that $h_i = h_i(p, x)$, as $i \in \{0, x, y, z\}$. For a wave function $\psi$, the Schrödinger equation gives

$$H\psi = E\psi$$  \hspace{1cm} (C.6)

$$(H - E\sigma_0)\psi = 0$$

$$(H - E\sigma_0)(e^{\eta \sigma_z/2} e^{-\eta \sigma_z/2})\psi = 0$$

$$e^{\eta \sigma_z/2}(H - E\sigma_0)e^{\eta \sigma_z/2}(N e^{-\eta \sigma_z/2}\psi) = 0$$

Here we pick $\sigma_z$, as we anticipate $h_0 \rightarrow -\mu(y)$ and $h_z \rightarrow B(y)$. Our goal will be to transform this chemical potential spatial dependence into a renormalized magnetic field. That is, we want to get rid of the identity $\sigma_0$ term, and modify the $h_z$ term. In the above we have added $N$ as a normalization constant for the new modified wave function. We write

$$\tilde{\psi} = N e^{-\eta \sigma_z/2}\psi$$  \hspace{1cm} (C.7)

The Schrödinger equation is

$$(e^{\eta \sigma_z/2} H e^{-\eta \sigma_z/2} - E e^{\eta \sigma_z/2} \sigma_0 e^{-\eta \sigma_z/2})\tilde{\psi} = 0$$  \hspace{1cm} (C.8)

$$[e^{\eta \sigma_z/2} H e^{-\eta \sigma_z/2} - E(\cosh(\eta)\sigma_0 + \sinh(\eta)\sigma_z)]\tilde{\psi} = 0$$

$$(e^{\eta \sigma_z/2} H e^{-\eta \sigma_z/2} - E \sinh(\eta)\sigma_z)\tilde{\psi} = E \cosh(\eta)\tilde{\psi}$$
Here we define
\[ \tilde{H} = e^{\eta \sigma_z/2} H e^{\eta \sigma_z/2} - E \sinh(\eta) \sigma_z \]  
(C.9)

This gives us
\[ \tilde{H} \tilde{\psi} = \cosh(\eta) E \tilde{\psi} \]  
(C.10)

We see that the first term of \( \tilde{H} \) can be written as
\[ e^{\eta \sigma_z/2} H e^{\eta \sigma_z/2} = h_0[\cosh(\eta) \sigma_0 + \sinh(\eta) \sigma_z] + h_x \sigma_x + h_y \sigma_y + h_z[\cosh(\eta) \sigma_z + \sinh(\eta) \sigma_0] \]  
(C.11)

Our goal is to remove the \( \sigma_0 \) dependence. Collecting the \( \sigma_0 \) terms in the above and setting them to zero, and defining \( \eta = \tanh^{-1} \beta \), we have
\[
\begin{align*}
    h_0 \cosh(\eta) + h_z \sinh(\eta) &= 0 \\
    h_0 \frac{1}{\sqrt{1 - \beta^2}} + h_z \frac{\beta}{\sqrt{1 - \beta^2}} &= 0 \\
    h_0 + h_z \beta &= 0 \\
    \beta &= \frac{h_0}{h_z}
\end{align*}
\]  
(C.12)
We note that this assumes $|h_0| < |h_z|$, as otherwise the denominators in the above would be complex. Choosing this value of $\beta$ gives

$$e^{\eta\sigma_z/2}He^{\eta\sigma_z/2} = h_0 \left[ \frac{1}{\sqrt{1 - \beta^2}} \sigma_0 + \frac{\beta}{\sqrt{1 - \beta^2}} \sigma_z \right]$$

$$+ h_x \sigma_x + h_y \sigma_y + h_z \left[ \frac{1}{\sqrt{1 - \beta^2}} \sigma_z + \frac{\beta}{\sqrt{1 - \beta^2}} \sigma_0 \right]$$

$$= h_0 \left[ \frac{1}{\sqrt{1 - (h_0/h_z)^2}} \sigma_0 - \frac{h_0/h_z}{\sqrt{1 - (h_0/h_z)^2}} \sigma_z \right]$$

$$+ h_x \sigma_x + h_y \sigma_y + h_z \left[ \frac{1}{\sqrt{1 - (h_0/h_z)^2}} \sigma_z - \frac{h_0/h_z}{\sqrt{1 - (h_0/h_z)^2}} \sigma_0 \right]$$

$$= h_x \sigma_x + h_y \sigma_y + \left[- \frac{h_0^2/h_z}{\sqrt{1 - (h_0/h_z)^2}} + \frac{h_z}{\sqrt{1 - (h_0/h_z)^2}} \right] \sigma_z$$

$$= h_x \sigma_x + h_y \sigma_y + h_z \left[ \frac{1 - (h_0/h_z)^2}{\sqrt{1 - (h_0/h_z)^2}} \right] \sigma_z$$

$$= h_x \sigma_x + h_y \sigma_y + h_z \sqrt{1 - (h_0/h_z)^2} \sigma_z$$

We see that the $h_z$ term gets renormalized. Now, the other term of $\tilde{H}$ becomes

$$E \sinh(\eta)\sigma_z = E \frac{\beta}{\sqrt{1 - \beta^2}} \sigma_z$$

$$= -E \frac{h_0/h_z}{\sqrt{1 - (h_0/h_z)^2}} \sigma_z$$

This gives us

$$\tilde{H} = e^{\eta\sigma_z/2}He^{\eta\sigma_z/2} - E \sinh(\eta)\sigma_z$$

$$= h_x \sigma_x + h_y \sigma_y + \left[ h_z \sqrt{1 - (h_0/h_z)^2} + E \frac{h_0/h_z}{\sqrt{1 - (h_0/h_z)^2}} \right] \sigma_z$$

Defining

$$\gamma = \frac{1}{\sqrt{1 - (h_0/h_z)^2}}$$

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We have

\[ \tilde{H} = h_x \sigma_x + h_y \sigma_y + \left[ \frac{h_z}{\gamma} - E \gamma \beta \right] \sigma_z \]  
(C.17)

\[ \tilde{H} \tilde{\psi} = \gamma E \tilde{\psi} \]  
(C.18)

Defining

\[ \tilde{h}_z = \frac{h_z}{\gamma} - E \gamma \beta \]  
(C.19)

We have

\[ \tilde{H} = h_x \sigma_x + h_y \sigma_y + \tilde{h}_z \sigma_z \]  
(C.20)

This can be written as

\[ \tilde{H} = \begin{pmatrix} \tilde{h}_z & h_x - ih_y \\ h_x + ih_y & -\tilde{h}_z \end{pmatrix} \]  
(C.21)

We anticipate that \( h_x \rightarrow \alpha p_y \), and \( h_0 \rightarrow -\mu(y) = -my \), and \( h_z \rightarrow B(y) = by \). To create ladder operators out of the \( p_y \) and \( y \) terms, we would like to rotate this Hamiltonian \( \tilde{H} \) such that \( h_x \) moves to the \( \sigma_y \) place and that \( \tilde{h}_z \) moves to the \( \sigma_x \) place. That is, we would like

\[ U^\dagger \tilde{H} U = h_x U^\dagger \sigma_x U + h_y U^\dagger \sigma_y U + \tilde{h}_z U^\dagger \sigma_z U \]  
(C.22)

\[ = h_x \sigma_y + h_y \sigma_z + \tilde{h}_z \sigma_x \]
This is to say, we want a unitary transformation which permutes the Pauli matrices, \( U^\dagger \sigma_i U = \sigma_{i+1} \), as \( i \in \{x, y, z\} \). This can be accomplished with the operator

\[
U = \frac{1}{\sqrt{2}} \left[ \frac{1 + i}{2} \left[ 1 - i \sigma_0 + \sigma_x + \sigma_y + \sigma_z \right] \right] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}
\]

(C.23)

Using this gives us

\[
U^\dagger \tilde{H} U = \begin{pmatrix} h_y & \tilde{h}_z - ih_x \\ \tilde{h}_z + ih_x & -h_y \end{pmatrix}
\]

(C.24)

C.2. Hyperbolic Transformations on 4×4 Hamiltonians

Adding a spatially varying chemical potential to our system studied in Chapter 4, our BdG Hamiltonian as written in Eq. (4.17) has the form

\[
\mathcal{H} = -\mu(y) \tau_z \sigma_0 + B(y) \tau_z \sigma_z + \alpha p_y \tau_0 \sigma_y - \alpha p_x \tau_z \sigma_y - \Delta \tau_y \sigma_y
\]

(C.25)

\[
= h_{z0} \tau_z \sigma_0 + h_{zz} \tau_z \sigma_z + h_{0x} \tau_0 \sigma_x + h_{zy} \tau_z \sigma_y + h_{yy} \tau_y \sigma_y
\]

We need to find a transformation which changes the \( h_{z0} \) and \( h_{zz} \) terms, while leaving all the other terms unchanged. Let us consider the hyperbolic transformation defined by \( e^{\eta \tau_0 \sigma_z / 2} \).
Calculating each example by hand, we find

\begin{align*}
  e^{\eta \sigma_z/2} \tau_z \sigma_0 e^{\eta \sigma_z/2} &= \cosh(\eta) \tau_z \sigma_0 + \sinh(\eta) \tau_z \sigma_z \\
  e^{\eta \sigma_z/2} \tau_z \sigma_z e^{\eta \sigma_z/2} &= \cosh(\eta) \tau_z \sigma_z + \sinh(\eta) \tau_z \sigma_0 \\
  e^{\eta \sigma_z/2} \tau_y \sigma_y e^{\eta \sigma_z/2} &= \tau_y \sigma_y \\
  e^{\eta \sigma_z/2} \tau_0 \sigma_x e^{\eta \sigma_z/2} &= \tau_0 \sigma_x \\
  e^{\eta \sigma_z/2} \tau_z \sigma_y e^{\eta \sigma_z/2} &= \tau_z \sigma_y \\
  e^{\eta \sigma_z/2} \tau_0 \sigma_0 e^{\eta \sigma_z/2} &= \cosh(\eta) \tau_0 \sigma_0 + \sinh(\eta) \tau_0 \sigma_z \\
  e^{\eta \sigma_z/2} \tau_0 \sigma_z e^{\eta \sigma_z/2} &= \cosh(\eta) \tau_0 \sigma_z + \sinh(\eta) \tau_0 \sigma_0
\end{align*}

We see the hyperbolic transformation defined by \( e^{\eta \sigma_z/2} \) modifies both the pair \((\tau_0 \sigma_0 \leftrightarrow \tau_0 \sigma_z)\) and the pair \((\tau_z \sigma_0 \leftrightarrow \tau_z \sigma_z)\), leaving all the other terms unmodified.

This may create some problems. We want to get rid of the \( h_{z0} \) term to get rid of the chemical potential, and rewrite the magnetic field in the \( h_{zz} \) term. However, the \( E \tau_0 \sigma_0 \) term in the definition of \( \tilde{H} \) will gain an \( \tau_0 \sigma_z \) term, which does not match up with any of the other terms in the BdG Hamiltonian. We will not simply have a redefined ladder operator, where the location of the wave function depends on energy, as in the previous section. We will obtain a more complicated matrix, which we will have to rewrite in another way.

We have that

\[
\mathcal{H} \Psi = E \Psi \tag{C.27}
\]

\[
(\mathcal{H} - E \tau_0 \sigma_0) \Psi = 0
\]

\[
e^{\eta \sigma_z/2} (\mathcal{H} - E \tau_0 \sigma_0) e^{\eta \sigma_z/2} (N e^{-\eta \sigma_z/2} \Psi) = 0
\]
Let \( \tilde{\Psi} = Ne^{-\eta_0 \sigma_z / 2} \Psi \) we have

\[
(e^{\eta_0 \sigma_z / 2} He^{\eta_0 \sigma_z / 2} - E^{\eta_0 \sigma_z}) \tilde{\Psi} = 0 \tag{C.28}
\]

\[
[e^{\eta_0 \sigma_z / 2} He^{\eta_0 \sigma_z / 2} - E(\cosh(\eta) \tau_0 \sigma_0 + \sinh(\eta) \tau_0 \sigma_z)] \tilde{\Psi} = 0
\]

\[
[e^{\eta_0 \sigma_z / 2} He^{\eta_0 \sigma_z / 2} - E \sinh(\eta) \tau_0 \sigma_z] \tilde{\Psi} = \cosh(\eta) E \tilde{\Psi}
\]

Let \( \mu(y) = my \) and \( B(y) = by \). We have that

\[
e^{\eta_0 \sigma_z / 2} H e^{\eta_0 \sigma_z / 2} = -\mu [\cosh(\eta) \tau_z \sigma_0 + \sinh(\eta) \tau_z \sigma_z] \tag{C.29}
\]

\[
+ B [\cosh(\eta) \tau_z \sigma_z + \sinh(\eta) \tau_z \sigma_0] + \alpha p_y \tau_0 \sigma_x - \alpha p_x \tau_z \sigma_y - \Delta \tau_y \sigma_y
\]

We want to remove all \( \tau_z \sigma_0 \) terms. Setting \( \eta = \tanh^{-1}(\beta) \), this requires

\[
-\mu \cosh(\eta) + B \sinh(\eta) = 0 \tag{C.30}
\]

\[
-\mu \frac{1}{\sqrt{1 - \beta^2}} + B \frac{\beta}{\sqrt{1 - \beta^2}} = 0
\]

\[
-\mu + B \beta = 0
\]

\[
\beta = \frac{\mu}{B} = \frac{m}{b}
\]

This assumes \( |m| < |b| \). This gives

\[
e^{\eta_0 \sigma_z / 2} H e^{\eta_0 \sigma_z / 2} = by \sqrt{1 - (m/b)^2} \tau_z \sigma_z + \alpha p_y \tau_0 \sigma_x - \alpha p_x \tau_z \sigma_y - \Delta \tau_y \sigma_y \tag{C.31}
\]

Let

\[
\tilde{\mathcal{H}} = e^{\eta_0 \sigma_z / 2} H e^{\eta_0 \sigma_z / 2} - \sinh(\eta) E \tau_0 \sigma_z \tag{C.32}
\]

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Then

\[
\tilde{\mathcal{H}} = by\sqrt{1 - (m/b)^2} \tau_z \sigma_z - E \frac{m/b}{\sqrt{1 - (m/b)^2}} \tau_0 \sigma_z + \alpha p_y \tau_0 \sigma_x - \alpha p_x \tau_z \sigma_y - \Delta \tau_y \sigma_y
\] (C.33)

Letting

\[
\gamma = \frac{1}{\sqrt{1 - (m/b)^2}}
\] (C.34)

we have

\[
\tilde{\mathcal{H}} = b \gamma y \tau_z \sigma_z - \gamma E \frac{m}{b} \tau_0 \sigma_z + \alpha p_y \tau_0 \sigma_x - \alpha p_x \tau_z \sigma_y - \Delta \tau_y \sigma_y
\] (C.35)

Writing

\[
\tilde{b} = \frac{b}{\gamma}
\] (C.36)

\[
\tilde{E} = \gamma E \frac{m}{b}
\] (C.37)

we have

\[
\tilde{\mathcal{H}} = \tilde{b} y \tau_z \sigma_z - \tilde{E} \tau_0 \sigma_z + \alpha p_y \tau_0 \sigma_x - \alpha p_x \tau_z \sigma_y - \Delta \tau_y \sigma_y
\] (C.38)

We will square this Hamiltonian, and then find the transformation which diagonalizes it.

Squaring the above Hamiltonian gives the result

\[
\tilde{\mathcal{H}}^2 = \left[ (by)^2 + \tilde{E}^2 + (\alpha p_y)^2 + (\alpha p_x)^2 + \Delta^2 \right] \tau_0 \sigma_0
\] (C.39)

\[
- 2 \tilde{E} by \tau_z \sigma_0 + \alpha \tilde{b} (y p_y - p_y y) \tau_z (i \sigma_y) - 2 \Delta \tilde{b} y (i \tau_x)(i \sigma_x)
\]
Recalling \([y, p_y] = i\hbar\), we have

\[
\tilde{H}^2 = \left[ (\tilde{b}y)^2 + \tilde{E}^2 + (\alpha p_y)^2 + (\alpha p_x)^2 + \Delta^2 \right] \tau_0 \sigma_0 - 2\tilde{E}\tilde{b}\tau_z \sigma_0 - \alpha \tilde{b}\tau_z \sigma_y + 2\Delta \tilde{b}\tau_z \sigma_x \quad \text{(C.40)}
\]

The eigenvectors of this object have the form

\[
\begin{pmatrix}
\frac{\tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\Delta} \\
\frac{-i \tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\Delta} \\
i \\
1
\end{pmatrix}, \quad \begin{pmatrix}
\frac{-\tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\Delta} \\
i \\
1
\end{pmatrix}, \quad \begin{pmatrix}
\frac{-\tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\Delta} \\
i \\
1
\end{pmatrix}, \quad \begin{pmatrix}
\frac{-\tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\Delta} \\
i \\
1
\end{pmatrix}
\]

\text{(C.41)}

We note that when \(\tilde{E} = 0\), this looks like \(U\) in Eq. (4.6). We can then make our transformation matrix out of these vectors, by using them as columns in the matrix. However, they first must be normalized. The first and third vectors have the magnitude

\[
\langle 1|1 \rangle = \left( \frac{\tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\Delta} \right)^2 + \left( \frac{-\tilde{E} + \sqrt{\tilde{E}^2 + \Delta^2}}{\Delta} \right)^2 + 1 + 1 = 4\frac{\tilde{E}^2 + \Delta^2 + \tilde{E}\sqrt{\tilde{E}^2 + \Delta^2}}{\Delta^2} \quad \text{(C.42)}
\]

The second and fourth vectors have the magnitude

\[
\langle 2|2 \rangle = 4\frac{\tilde{E}^2 + \Delta^2 - \tilde{E}\sqrt{\tilde{E}^2 + \Delta^2}}{\Delta^2} \quad \text{(C.43)}
\]

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The normalization coefficients are then

\[
N = \frac{1}{2} \frac{\Delta}{\sqrt{E^2 + \Delta^2 \pm \tilde{E}\sqrt{E^2 + \Delta^2}}} \tag{C.44}
\]

Normalizing each of our vectors, we obtain our transformation matrix as

\[
W = \begin{pmatrix}
    \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}} \\
    \frac{i}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{i}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{i}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{i}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}} \\
    \frac{i}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{i}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{i}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{i}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}} \\
    \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 - \tilde{E}\sqrt{E^2 + \Delta^2}}} & \frac{-\tilde{E} + \sqrt{E^2 + \Delta^2}}{\sqrt{E^2 + \Delta^2 + \tilde{E}\sqrt{E^2 + \Delta^2}}}
\end{pmatrix} \tag{C.45}
\]

We have that \(W^\dagger W = \tau_0\sigma_0\). We also can find that when \(\tilde{E} = 0\), we have

\[
W|_{\tilde{E}=0} = U \tag{C.46}
\]

As \(U\) is defined in Eq. (4.6). Rotating the squared Hamiltonian gives

\[
W^\dagger \tilde{H}^2 W = \text{diag}((\alpha p_x)^2 + (\alpha p_y)^2 + \tilde{b}^2(y - \sqrt{\frac{E^2 + \Delta^2}{b}})^2 - \alpha \tilde{b} \hbar, \tag{C.47}
\]

\[
(\alpha p_x)^2 + (\alpha p_y)^2 + \tilde{b}^2(y + \sqrt{\frac{E^2 + \Delta^2}{b}})^2 - \alpha \tilde{b} \hbar,
\]

\[
(\alpha p_x)^2 + (\alpha p_y)^2 + \tilde{b}^2(y - \sqrt{\frac{E^2 + \Delta^2}{b}})^2 + \alpha \tilde{b} \hbar,
\]

\[
(\alpha p_x)^2 + (\alpha p_y)^2 + \tilde{b}^2(y + \sqrt{\frac{E^2 + \Delta^2}{b}})^2 + \alpha \tilde{b} \hbar)
\]

We see that these entries look like Harmonic Oscillator equations, with the center of the wave functions shifted by \(\sqrt{\tilde{E}^2 + \Delta^2}/\tilde{b}\). Performing this same rotation on the Hamiltonian
itself, we find

\[
W^\dagger \hat{H} W = \begin{pmatrix}
-\alpha p_x & 0 & \sqrt{2abha}^\dagger & 0 \\
0 & -\alpha p_x & 0 & \sqrt{2abha}^\dagger \\
\sqrt{2abha}_- & 0 & \alpha p_x & 0 \\
0 & \sqrt{2abha}_+ & 0 & \alpha p_x \\
\end{pmatrix}
\] (C.48)

Here we have defined the ladder operators

\[
a_\pm = \sqrt{\frac{\tilde{b}}{2\alpha \hbar}} \left[ \left( y \pm \frac{\sqrt{E^2 + \Delta^2}}{\tilde{b}} \right) + i \frac{\alpha}{\tilde{b} p_y} \right]
\] (C.49)

This object is analogous to what we have studied before. We see that the effect of the electric field is to redefine the parameter \( \tilde{b} \) and to shift the position of the ladder operators and wave functions.
Appendix D. Bound State Solutions in Circular Geometries

In this appendix we analytically derive the Majorana bound state wave functions studied in Chapter 5. We consider a two-dimensional superconductor held at a constant Zeeman exchange energy, and introduce a circular nanoflake which creates an inhomogenous chemical potential. Letting \( R_0 \) be the radius of the nanoflake, we assume that the chemical potential is given by

\[
\mu(r) = \begin{cases} 
\mu_1 & r < R_0 \\
\mu_2 & r > R_0 
\end{cases}.
\]

Our goals are to obtain the bound state solutions localized at \( r = R_0 \), and to obtain their energy eigenvalues. Let us define the Hamiltonians \( H_1(r, \nabla) \) and \( H_2(r, \nabla) \) for \( r < R_0 \) and \( r > R_0 \), respectively. We have

\[
H_1(r, \nabla) = -\mu_1 \sigma_0 + \alpha (\sigma \times -i\nabla)_z + h\sigma_z,
\]

\[
H_2(r, \nabla) = -\mu_2 \sigma_0 + \alpha (\sigma \times -i\nabla)_z + h\sigma_z.
\]

Here the system is two-dimensional with \( r = (x, y) \). To proceed, we shall then analyze each Hamiltonian separately, and then match their wave function solutions at the \( r = R_0 \) boundary.

D.1. Wave Function as \( r < R_0 \)

Let us first focus on \( H_1(r, \nabla) \). The second quantized real-space Bogoliubov-de Gennes Hamiltonian is given by

\[
\mathcal{H}_1 = \frac{1}{2} \int dr \Psi^\dagger(r) \begin{pmatrix} H_1(r, \nabla) & i\sigma_y \Delta \\
-i\sigma_y \Delta & -H_1^T(r, -\nabla) \end{pmatrix} \Psi(r).
\]

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Here $\Psi(\mathbf{r}) = (\psi_\uparrow(\mathbf{r}), \psi_\downarrow(\mathbf{r}), \psi_\uparrow^\dagger(\mathbf{r}), \psi_\downarrow^\dagger(\mathbf{r}))^T$, where $\psi_\sigma(\mathbf{r})$ are electron field operators which destroy an electron at location $\mathbf{r}$. We have that

$$\mathcal{H}_1 = \frac{1}{2} \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \begin{pmatrix} -\mu_1 + h & \alpha e^{-i\theta} (\partial_r - i\frac{1}{r} \partial_\theta) & 0 & \Delta \\ \alpha e^{i\theta} (-\partial_r - i\frac{1}{r} \partial_\theta) & -\mu_1 - h & -\Delta & 0 \\ 0 & -\Delta & \mu_1 - h & \alpha e^{i\theta} (-\partial_r - i\frac{1}{r} \partial_\theta) \\ \Delta & 0 & \alpha e^{-i\theta} (\partial_r - i\frac{1}{r} \partial_\theta) & \mu_1 + h \end{pmatrix} \Psi(\mathbf{r})$$

$$= \frac{1}{2} \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \mathcal{H}_1 \Psi(\mathbf{r}).$$

We then wish to find the eigenvectors of $\mathcal{H}_1$. That is, we wish to find eigenvectors $\varphi$ such that $\mathcal{H}_1 \varphi = E \varphi$. Consider the total angular momentum operator,

$$J_z = -i \partial_\theta \tau_0 \sigma_0 + \frac{1}{2} \tau_z \sigma_z.$$

We can verify that this operator commutes with the first quantized Hamiltonian, $[J_z, \mathcal{H}_1] = 0$. Thus, the Hamiltonian $\mathcal{H}_1$ and the total angular momentum operator $J_z$ have the same eigenstates. The eigenstates of $J_z$ are given by

$$\varphi_n = \begin{pmatrix} u_{n\uparrow}(r) e^{i(n-1)\theta} \\ u_{n\downarrow}(r) e^{i\theta} \\ v_{n\uparrow}(r) e^{i\theta} \\ v_{n\downarrow}(r) e^{i(n-1)\theta} \end{pmatrix}.$$  

Here $n$ is an integer, $n \in \mathbb{Z}$, and we may verify that

$$J_z \varphi_n = \left(n - \frac{1}{2}\right) \varphi_n = m_J \varphi_n.$$  

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Note that the eigenvalues of $J_z$ are half-integer, given by $m_J = n - \frac{1}{2}$. From the expression $H_1 \varphi_n = E \varphi_n$ we then obtain the system of equations,

$$
(-\mu_1 + h)u_{n\uparrow}(r) + \alpha \left[ \partial_r + \frac{n}{r} \right] u_{n\downarrow}(r) + \Delta v_{n\downarrow}(r) = Eu_{n\uparrow}(r),
$$

$$\alpha \left[ -\partial_r + \frac{n - 1}{r} \right] u_{n\downarrow}(r) + (-\mu_1 - h)u_{n\uparrow}(r) - \Delta v_{n\uparrow}(r) = Eu_{n\downarrow}(r), \quad (D.8)$$

Now, we expect to find a localized state at $r = R_0$, which decays as $r \to 0$ and $r \to \infty$. That is, for the $r < R_0$ region, we expect the $\{u\}$ and $\{v\}$ functions to be related to the modified Bessel functions of the first kind $I_n(kr)$, which are finite as $r = 0$. Here, $k$ is the radial momentum. The modified Bessel functions of the first kind obey the following recurrence relations:

$$\frac{n}{kr} I_n(kr) = \frac{1}{2} \left( I_{n-1}(kr) - I_{n+1}(kr) \right), \quad (D.9)$$

$$\partial_{kr} I_n(kr) = \frac{1}{2} \left( I_{n-1}(kr) + I_{n+1}(kr) \right). \quad (D.10)$$

From these, we may find that

$$
\left[ \partial_r + \frac{n}{r} \right] I_n(kr) = kI_{n-1}(kr), \quad (D.11)
$$

$$\left[ -\partial_r + \frac{n - 1}{r} \right] I_{n-1}(kr) = -kI_n(kr).$$
Let us then assume that our vector has the form

$$\varphi_n = \begin{pmatrix} aI_{n-1}(kr) e^{i(n-1)\theta} \\
bI_n(kr) e^{in\theta} \\
cI_n(kr) e^{in\theta} \\
dI_{n-1}(kr) e^{i(n-1)\theta} \end{pmatrix}. \quad \text{(D.12)}$$

With this assumption, our system of equations then has the form

$$\begin{align*}
(-\mu_1 + h)a + \alpha kb + \Delta d &= Ea, \\
-\alpha ka + (-\mu_1 - h)b - \Delta c &= Eb, \\
-\Delta b + (\mu_1 - h)c - \alpha kd &= Ec, \\
\Delta a + \alpha kc + (\mu_1 + h)d &= Ed.
\end{align*} \quad \text{(D.13)}$$

$$\begin{pmatrix}
-\mu_1 + h - E & \alpha k & 0 & \Delta \\
-\alpha k & -\mu_1 - h - E & -\Delta & 0 \\
0 & -\Delta & \mu_1 - h - E & -\alpha k \\
\Delta & 0 & \alpha k & \mu_1 + h - E
\end{pmatrix}
\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} =
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad \text{(D.14)}$$

Setting the determinant to zero gives

$$k_\pm = \frac{1}{\alpha} \sqrt{h^2 - E^2 + \Delta^2 - \mu_1^2 \pm 2\sqrt{E^2\mu_1^2 + \Delta^2(h - \mu_1)(h + \mu_1)}}, \quad \text{(D.15)}$$
and

\[ a_\pm = \frac{-E \mu_1 \pm \sqrt{h^2 \Delta^2 + (E - \Delta)(E + \Delta) \mu_1^2}}{\Delta(h - \mu_1)}, \quad \text{(D.16)} \]

\[ b_\pm = (E \mu_1 \mp \sqrt{h^2 \Delta^2 + (E - \Delta)(E + \Delta) \mu_1^2}) \]

\[ \times \frac{\sqrt{h^2 - E^2 + \Delta^2 - \mu_1^2 \pm 2 \sqrt{E^2 \mu_1^2 + \Delta^2 (h - \mu_1)(h + \mu_1)}}}{\Delta[h(h + E) - \mu_1^2 \pm \sqrt{h^2 \Delta^2 + (E - \Delta)(E + \Delta) \mu_1^2}]}, \quad \text{(D.17)} \]

\[ c_\pm = -\frac{(h + \mu_1)\sqrt{h^2 - E^2 + \Delta^2 - \mu_1^2 \pm 2 \sqrt{E^2 \mu_1^2 + \Delta^2 (h - \mu_1)(h + \mu_1)}}}{h(h + E) - \mu_1^2 \pm \sqrt{h^2 \Delta^2 + (E - \Delta)(E + \Delta) \mu_1^2}}, \quad \text{(D.18)} \]

\[ d_\pm = 1. \quad \text{(D.19)} \]

The wave function as \( r < R_0 \) then has the generic form,

\[ \varphi_n(r) = N_n^+ \left( \begin{array}{c}
    a_+ I_{n-1}(k_+ r) e^{i(n-1)\theta} \\
    b_+ I_n(k_+ r) e^{in\theta} \\
    c_+ I_n(k_+ r) e^{in\theta} \\
    I_{n-1}(k_+ r) e^{i(n-1)\theta}
  \end{array} \right) + N_n^- \left( \begin{array}{c}
    a_- I_{n-1}(k_- r) e^{i(n-1)\theta} \\
    b_- I_n(k_- r) e^{in\theta} \\
    c_- I_n(k_- r) e^{in\theta} \\
    I_{n-1}(k_- r) e^{i(n-1)\theta}
  \end{array} \right). \quad \text{(D.20)} \]

Here \( N_n^\pm \) are normalization constants.

**D.2. Wave Function as \( r > R_0 \)**

We can then repeat this analysis for the region \( r > R_0 \). The analysis will then be the same, except that the chemical potential will be given by \( \mu_2 \). In the \( r > R_0 \) region, the wave function must decay as \( r \to \infty \). Thus, we must use the modified Bessel functions of the second kind \( K_n(kr) \). However, these objects do not satisfy the same recurrence relations. Instead, the object \( e^{i\pi K_n(kr)} \) satisfies the following recurrence relations:

\[ \frac{n}{kr} [e^{i\pi K_n(kr)}] = \frac{1}{2} \left( e^{i(n-1)\pi K_{n-1}(kr)} - e^{i(n+1)\pi K_{n+1}(kr)} \right), \quad \text{(D.21)} \]

\[ \partial_r [e^{i\pi K_n(kr)}] = \frac{1}{2} \left( e^{i(n-1)\pi K_{n-1}(kr)} + e^{i(n+1)\pi K_{n+1}(kr)} \right). \]

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From these, we may find that

$$\left[ \partial_r + \frac{n}{r} \right] e^{i\pi} K_n(kr) = ke^{i(n-1)\pi} K_{n-1}(kr), \quad (D.22)$$

and

$$\left[ -\partial_r + \frac{n-1}{r} \right] e^{i(n-1)\pi} K_{n-1}(kr) = -ke^{i\pi} K_n(kr). \quad (D.23)$$

Following similar steps as in the previous section, we may find that the wave function then has the form,

$$\tilde{\varphi}_n(r) = \tilde{N}_n^+ \begin{pmatrix} \tilde{a}_+ e^{i(n-1)\pi} K_{n-1}(\tilde{k}_+ r) e^{i(n-1)\theta} \\ \tilde{b}_+ e^{i\pi} K_n(\tilde{k}_+ r) e^{in\theta} \\ \tilde{c}_+ e^{i\pi} K_n(\tilde{k}_+ r) e^{in\theta} \\ e^{i(n-1)\pi} K_{n-1}(\tilde{k}_+ r) e^{i(n-1)\theta} \end{pmatrix} + \tilde{N}_n^- \begin{pmatrix} \tilde{a}_- e^{i(n-1)\pi} K_{n-1}(\tilde{k}_- r) e^{i(n-1)\theta} \\ \tilde{b}_- e^{i\pi} K_n(\tilde{k}_- r) e^{in\theta} \\ \tilde{c}_- e^{i\pi} K_n(\tilde{k}_- r) e^{in\theta} \\ e^{i(n-1)\pi} K_{n-1}(\tilde{k}_- r) e^{i(n-1)\theta} \end{pmatrix}. \quad (D.24)$$

Here the parameters \{\tilde{k}_\pm, \tilde{a}_\pm, \tilde{b}_\pm, \tilde{c}_\pm\} have the same form as those given in the previous section, except that we replace \(\mu_1 \to \mu_2\).

### D.3. Expression for the Bound State Energy

Matching the wave functions at \(r = R_0\), we obtain \(\varphi_n(R_0) = \tilde{\varphi}_n(R_0)\). This expression gives us the system of equations,

$$N_n^+ a_+ I_{n-1}(k_+ R_0) + N_n^- a_- I_{n-1}(k_- R_0) = \tilde{N}_n^+ \tilde{a}_+ e^{i(n-1)\pi} K_{n-1}(\tilde{k}_+ R_0)$$

$$+ \tilde{N}_n^- \tilde{a}_- e^{i(n-1)\pi} K_{n-1}(\tilde{k}_- R_0),$$

$$N_n^+ b_+ I_n(k_+ R_0) + N_n^- b_- I_n(k_- R_0) = \tilde{N}_n^+ \tilde{b}_+ e^{i\pi} K_n(\tilde{k}_+ R_0) + \tilde{N}_n^- \tilde{b}_- e^{i\pi} K_n(\tilde{k}_- R_0),$$

$$N_n^+ c_+ I_n(k_+ R_0) + N_n^- c_- I_n(k_- R_0) = \tilde{N}_n^+ \tilde{c}_+ e^{i\pi} K_n(\tilde{k}_+ R_0) + \tilde{N}_n^- \tilde{c}_- e^{i\pi} K_n(\tilde{k}_- R_0),$$

$$N_n^+ I_{n-1}(k_+ R_0) + N_n^- I_{n-1}(k_- R_0) = \tilde{N}_n^+ \tilde{e}^{i(n-1)\pi} K_{n-1}(\tilde{k}_+ R_0) + \tilde{N}_n^- \tilde{e}^{i(n-1)\pi} K_{n-1}(\tilde{k}_- R_0). \quad (D.25)$$

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This is then a transcendental equation which must be numerically solved for the energy to zero. Finding the determinant and setting it to zero, we then obtain the expression,

\[
\begin{pmatrix}
  a_+ I_{n-1}(k_+ R_0) & a_- I_{n-1}(k_- R_0) & -\tilde{a}_+ e^{i(n-1)\pi} K_{n-1}(\tilde{k}_+ R_0) & -\tilde{a}_- e^{i(n-1)\pi} K_{n-1}(\tilde{k}_- R_0) \\
  b_+ I_{n}(k_+ R_0) & b_- I_{n}(k_- R_0) & -\tilde{b}_+ e^{in\pi} K_n(\tilde{k}_+ R_0) & -\tilde{b}_- e^{in\pi} K_n(\tilde{k}_- R_0) \\
  c_+ I_{n}(k_+ R_0) & c_- I_{n}(k_- R_0) & -\tilde{c}_+ e^{in\pi} K_n(\tilde{k}_+ R_0) & -\tilde{c}_- e^{in\pi} K_n(\tilde{k}_- R_0) \\
  I_{n-1}(k_+ R_0) & I_{n-1}(k_- R_0) & -e^{i(n-1)\pi} K_{n-1}(\tilde{k}_+ R_0) & -e^{i(n-1)\pi} K_{n-1}(\tilde{k}_- R_0)
\end{pmatrix}
\times
\begin{pmatrix}
  N^+_n \\
  N^-_n \\
  \tilde{N}^+_n \\
  \tilde{N}^-_n
\end{pmatrix} = 0.
\]

(D.26)

In order to have a nontrivial bound state, the determinant of the above matrix must be equal to zero. Finding the determinant and setting it to zero, we then obtain the expression,

\[
I_n(k_- R_0) \left\{ - (\tilde{a}_- - \tilde{a}_+)(b_+ c_+ - b_- c_-) I_n(k_+ R_0) K_n(\tilde{k}_+ R_0) K_{n-1}(\tilde{k}_- R_0) K_{n-1}(\tilde{k}_+ R_0) \\
+ I_{n-1}(k_+ R_0) \left[ (-a_+ + \tilde{a}_+)(\tilde{b}_- c_- - b_- \tilde{c}_-) K_{n-1}(\tilde{k}_+ R_0) K_n(\tilde{k}_- R_0) \\
+ (\tilde{a}_- + a_+)(\tilde{b}_+ c_- - b_- \tilde{c}_+) K_{n-1}(\tilde{k}_- R_0) K_n(\tilde{k}_+ R_0) \right] \right\} \\
+ I_{n-1}(k_- R_0) \left\{ (-a_- + a_+)(\tilde{b}_+ \tilde{c}_- - \tilde{b}_- \tilde{c}_+) I_{n-1}(k_+ R_0) K_n(\tilde{k}_- R_0) K_n(\tilde{k}_+ R_0) \\
+ I_n(k_+ R_0) \left[ (-a_- + a_+)(b_+ \tilde{c}_- - b_- \tilde{c}_+) K_{n-1}(\tilde{k}_+ R_0) K_n(\tilde{k}_- R_0) \\
+ (a_- + \tilde{a}_-)(\tilde{b}_+ c_+ - b_+ \tilde{c}_+) K_{n-1}(\tilde{k}_- R_0) K_n(\tilde{k}_+ R_0) \right] \right\} = 0.
\]

(D.27)

This is then a transcendental equation which must be numerically solved for the energy \( E \).
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Proximity-induced superconductivity at non-helical topological insulator interfaces


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Volkov-Pankratov states in topological superconductors

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David James Alspaugh was born in La Jolla, California. He attended the University of California, Berkeley, where he received a Bachelor of Arts degree in Physics and Pure Mathematics as a double major in May 2015. Immediately following college, he began his graduate studies at Louisiana State University in analytical condensed matter theory. He looks forward to continuing his work in condensed matter physics as a postdoctoral researcher at California State University, Northridge.