

Thesis

Novel topological superconductivity
and bulk-boundary correspondence

Akito Daido

Department of Physics, Kyoto University

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Abstract

Topological superconductivity and bulk-boundary correspondence are among the central topics in modern condensed matter physics. Stimulated by the proposal to use Majorana fermions as qubits of topological quantum computation [1], about two decades of research has revealed that topological superconductivity may be realized in systems such as nanowires and doped topological insulators [2]. Now we can say that topological superconductivity, as well as bulk-boundary correspondence in superconductors, begins to be accepted as a material phase in nature. Therefore, one of the next steps of theoretical research is to investigate a variety of topological superconductivity and bulk-boundary correspondence. Based on this background, in this thesis, we focus on two novel aspects of topology in superconductors [3, 4].

First, we study the interplay of topological superconductivity and crystalline symmetries. In particular, we focus on non-symmorphic symmetries, whose symmetry operations consist of point-group operation and fractional-lattice translation. It has been pointed out that the non-symmorphic glide symmetry gives rise to an intriguing topological (crystalline) superconductivity classified into $\mathbb{Z}_4$ topological phases [5], which do not appear in conventional topological periodic table of Altland-Zirnbauer classes [6, 7, 8]. However, material candidate for the $\mathbb{Z}_4$ topological superconductivity has not been known. We reveal that the paramagnetic superconducting phase of UCoGe is the first promising material candidate of (first-order) $\mathbb{Z}_4$ topological crystalline superconductivity, as well as the second candidate of $\mathbb{Z}_2$ topological nonsymmorphic crystalline superconductivity. We derive Fermi-surface formulas predicting $\mathbb{Z}_4$ and $\mathbb{Z}_2$ topological invariants ensured by the glide symmetry, for the space group $Pnma$. We identify UCoGe as $\mathbb{Z}_4$ and $\mathbb{Z}_2$ topological crystalline superconductivity, by applying the formulas to the Fermi surfaces previously obtained by first-principles calculations [9, 10, 11].

Second, we consider a novel bulk-boundary correspondence in chiral symmetric systems. Examples include Kitaev chain [1], Majorana nanowires [12, 13], and time-reversal symmetric superconductors. In usual bulk-boundary correspondence, the integer-valued topological invariants predict the number of boundary states. Thus, the correspondence is between two integers defined in the bulk and the boundary. Recently, it has been proposed that this relation can be generalized to the correspondence between two continuous functions defined in the bulk and the boundary, in one-dimensional chiral symmetric systems [14]. In the context

of superconductivity, this relation, named spectral bulk-boundary correspondence (SBBC), means that surface accumulation of odd-frequency Cooper pairs are given by a bulk quantity named generalized winding number (both of them are functions of frequency). However, original proposal was the conjecture based on the observation of a number of numerical calculations, and formal proof of SBBC has been lacking. We point out that an analogy holds between SBBC and electric polarization: SBBC can be understood as the polarization of chirality. We give two proofs of SBBC based on this idea.

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List of publications

Papers related to the thesis

1. Akito Daido, Tsuneya Yoshida and Youichi Yanase,
 $\mathbb{Z}_4$ Topological Superconductivity in UCoGe,
Phys. Rev. Lett. **122**, 227001 (2019).
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2. Akito Daido and Youichi Yanase,
Chirality polarizations and spectral bulk-boundary correspondence,
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Chapter 1

Introduction to topological superconductivity

These days, topology plays more and more important roles in understanding properties of superconductors. Historically, superconductivity has been classified mainly by symmetry of Cooper pairs [15], until the advent of topology. Topology offers us a novel view point: We can understand a superconductor not only by what the pairing symmetry is, but also by whether it is topological or not. Superconductivity with nontrivial topological structure in the quasiparticle wave functions is called *topological superconductivity* [2, 16, 17, 18]. The study of topological superconductivity is one of the central topics in modern condensed matter physics. In this chapter, we make a brief introduction to topological superconductivity.

1.1 Topological superconductivity: an overview

In this section, we overview the research field of topological superconductivity.

1.1.1 Topological superconductivity

Originally, topological properties of materials were discussed in gapful systems such as insulators and superconductors, based on the dimensions and the local symmetries of the system. The results are summarized into a table known as the topological periodic table [6, 7, 8]. In the topological periodic table, a system is classified into one of the ten Altland-Zirnbauer classes, which is identified by the presence or absence of time-reversal, particle-hole, and chiral symmetries. For example, (spinful) superconductors with and without time-reversal symmetry correspond to class DIII and D, respectively. In particular, two-dimensional (2D) chiral superconductivity belongs to the class D, which has only the particle-hole symmetry, and is characterized by an integer (*topological invariant*) called the Chern number [19, 20]. It

is well known that spinless chiral p -wave superconductor with single Fermi surface has Chern number 1, and is a prototypical example of topological superconductivity [21].

As a result of the nontrivial topological invariants in the bulk, there appear zero-energy states at system boundaries. The prediction of surface states based on the topological invariants, a bulk property, is called *bulk-boundary correspondence* [22], and is one of the important properties of topological materials. Intuitively, the number of gapless surface states seems to be dependent on the details of surfaces, but it is not in reality. In this sense, bulk-boundary correspondence is an intriguing relation, and is worthy of investigation.

1.1.2 Experimental platforms

Topological superconductivity is also known as a promising platform to realize Majorana fermions with non-Abelian statistics. It has been proposed that Majorana fermions can be used as a building block of topological quantum computation [1, 18]. This fact has strongly motivated experimentalists to realize topological superconductivity. In the following, we introduce only a part of experimental results. We refer the readers to Refs. [2, 18] for a comprehensive review of topological superconductors.

In general, topologically nontrivial structure requires complex wave-number dependence of quasiparticle wave functions. This fact naturally makes unconventional superconductors the best candidate of topological superconductivity, since they have anisotropic order parameters. In this sense, the platforms of topological superconductivity might be categorized into the following two: either *artificial* or *intrinsic* unconventional superconductivity.

The first strategy to obtain topological superconductivity is to *engineer* a system similar to unconventional superconductivity. In particular, spinless chiral p -wave superconductivity is known to host single Majorana fermion, which is advantageous for application. Thus, the mainstream of the research has been the engineering of the effective spinless chiral p -wave superconductivity. One of the central platforms is the proximity-induced topological superconductivity in the heterostructures of semiconductor nanowire and s -wave superconductor [12, 13]. It has been theoretically shown that s -wave superconductivity with Rashba spin-orbit coupling and large Zeeman field becomes topologically nontrivial when chemical potential is fine-tuned to the Dirac point of the Rashba system [12, 13, 23, 24, 25]. Owing to the intensive experimental effort, signatures of Majorana fermion such as zero-bias conductance peak have already been reported [26, 27, 28, 29]. Theoretical and experimental efforts have also been made in other systems such as the heterostructures of quantum anomalous Hall insulator and s -wave superconductor [30, 31, 32, 33], as well as of topological insulator and s -wave superconductor [34, 35, 36, 37, 38]. There is also an attempt to realize the latter state within a single superconductor whose normal state is topological semimetal [39, 40, 41, 42, 43].

The second platform is, of course, those superconductors that intrinsically show unconven-

tional superconducting phases. Compared with the artificial topological superconductivity, they may not be a good platform of topological quantum computation due to the complexity of strongly-correlated materials as well as possible nodal excitations. Nevertheless, they are precious platforms of topological superconductivity which allow us to study topological view of superconductors. One of the important advantages of intrinsic superconductors is the presence of crystalline symmetries. As we introduce in the subsequent subsections, the interplay of topological superconductivity with crystalline symmetries gives rise to an interesting topological phase called *topological crystalline superconductivity*. Thus, intrinsic unconventional superconductors provide a fertile playground to pursue novel topology realized in nature.

Among various intrinsic unconventional superconductors, chiral superconductors [44], whose pair potential breaks time-reversal symmetry, are considered to be a good platform of class D topological superconductivity as well as Weyl superconductivity [45]. Material candidates include URu_2Si_2 [44], Sr_2RuO_4 [46, 47, 48], and UPt_3 [49, 50, 51, 52], where possibility of topological crystalline superconductivity is also discussed for the latter two [48, 50, 52]. Ferromagnetic superconductors UCoGe , URhGe , UGe_2 [53, 54] are also the promising candidates, because ferromagnetism is naturally expected to induce chiral order parameter. They are also candidates of odd-parity spin-triplet superconductivity, which is advantageous to obtain nontrivial topology. Recently discovered paramagnetic superconducting phase of UTe_2 at ambient pressure [55] is a promising candidate of spin-triplet superconductor with nontrivial topological invariants of class DIII [56]. An important material family of candidate class-DIII topological superconductors is the superconducting topological materials such as $\text{Cu}_x\text{Bi}_2\text{Se}_3$ [2, 57, 58, 59, 60]. A signature of zero-energy surface states has been reported by scanning-tunneling microscopy (STM) [61]. Further experimental study is awaited to fully establish topological superconductivity in these intrinsic unconventional superconductors.

1.1.3 Recent developments

After about two decades of research, topological properties are recognized to appear in a broader context of superconductors. Recent developments in the research field of topological superconductivity might be summarized into the following three directions.

Interplay with crystalline symmetries. It has been shown that crystalline symmetries enrich the topological structure of materials. Topologically nontrivial superconductivity whose topological nature is ensured by crystalline symmetries is called *topological crystalline superconductivity*. We discuss the details of topological crystalline superconductivity in the next subsection, since this is one of the main topics of this thesis (discussed in Chapter 2).

Topology in gapless superconductors. It has been clarified that gapless systems may also have topological properties. By considering lines or surfaces in three dimensional

Brillouin zone, one-dimensional or two-dimensional gapful systems, respectively, are effectively obtained, as long as gapless excitations are absent there. Accordingly, topological invariants are well-defined and gapless boundary states are ensured by bulk-boundary correspondence. In the context of superconductivity, Andreev bound states of d -wave superconductors (with line nodes) are shown to be protected by the topological invariant of 1D class AIII systems (the winding number) [62, 63, 64]. Now it is usual to call these gapless superconductivity with topologically nontrivial structure as ‘topological superconductivity’ as well.

The surface states in gapless superconductors mentioned above are closely related to the bulk excitation nodes. It can be said that in d -wave superconductors, the topological invariant of 1D class AIII systems, in turn, protects the line nodes. In general, the presence of excitation nodes in superconductors is ensured by some topological invariants.¹ Another example is the Weyl superconductivity [45] realized in superconductors breaking time-reversal symmetry, where point nodes are protected by the Chern number, accompanying surface Majorana arcs connecting two Weyl points. Comprehensive classification of excitation nodes in superconductors based on the concept of topology is now under progress (see e.g. Ref. [65] and references therein), where crystalline symmetries also play essential roles.

Extension of the concept of bulk-boundary correspondence. In usual bulk-boundary correspondence, topology of d -dimensional bulk system predicts gapless states on the $d - 1$ -dimensional boundaries. Recently, it has been shown that the concept of bulk-boundary correspondence can be generalized to higher-order ones [66, 67, 68, 69, 70]: In n -th order topological insulators and superconductors, gapless states appear on the $d - n$ dimensional boundaries in finite-sized systems. For example, three-dimensional (3D) second order topological superconductivity hosts Majorana *hinge* states, in contrast to the usual (i.e. first-order) 3D topological superconductivity which hosts Majorana *surface* states. Possibility and realization of higher-order topological superconductivity in real materials are one of the important future directions. So far, higher-order topological superconductivity has been proposed in, for example, iron-based superconductors [71, 72].

Apart from the research of higher-order topological phases, we note that there is another effort to enlarge the concepts of bulk-boundary correspondence. Recently, it has been suggested by numerics that the topological bulk-boundary correspondence in 1D chiral symmetric systems (such as time-reversal symmetric superconductivity) can be generalized to a *continuous* correspondence of the quantities defined in the bulk and

¹To be precise, we do not have a proof of this statement, but counter-example is not known to the best of our knowledge.

surface, with a surprising robustness against surface disorders [14]. This is an interesting relation, but their proposal is based on numerical illustrations and lacks a formal proof. We prove the continuous correspondence in Chapter 3.

1.1.4 Topological crystalline superconductivity

In this subsection, we briefly introduce topological crystalline superconductivity. Topological crystalline superconductivity refers to a kind of topological superconductivity where crystalline symmetries play an essential role. The basic idea might be seen in topological mirror superconductivity, whose topological structure is protected by the mirror symmetry [73]. When we consider mirror-invariant planes in 3D Brillouin zone, Hamiltonian is diagonalized with the mirror operator. Thus, we can define topological invariants such as the Chern number within each mirror sector. The difference of the two mirror-sector Chern numbers is called the mirror Chern number, which is independent of the usual Chern number given by the summation of the two mirror-sector Chern numbers. In this way, crystalline symmetries generally impose constraints on the structure of Hamiltonian, which enables us to define additional topological invariants.

Topological crystalline superconductivity also shows bulk-boundary correspondence. The difference from the usual topological superconductivity is that boundary states appear only on the surfaces preserving the relevant crystalline symmetry. Although the impurity effects on the surface states of topological crystalline superconductivity has not been studied well, they may be stable against disorder preserving the relevant symmetries on average [2], as evidenced for weak topological insulators and topological crystalline insulators [74, 75, 76, 77, 78].

Reflecting various crystalline symmetries, there are a variety of topological crystalline superconductivity [48, 50, 51, 52, 73, 79, 80, 81, 82, 83, 84]. In particular, complete classification of order-two crystalline symmetries has been obtained [5, 81], and some of the topological crystalline superconductivity (including higher-order ones) can be easily identified with the symmetry indicators [85, 86, 87, 88]. Among various classes of topological crystalline superconductivity, those protected by non-symmorphic crystalline symmetries are called topological nonsymmorphic crystalline superconductivity [5, 52, 89, 90]. Here, nonsymmorphic crystalline symmetry is a symmetry given by point-group operation followed by a fractional-lattice translation, and exists in 157 out of 230 space groups. For example, the operation of glide symmetry consists of a mirror operation and a half-lattice translation. In this thesis, we call topological nonsymmorphic crystalline superconductivity protected by glide symmetry as *topological glide superconductivity*.

One of the characteristics of the topological glide superconductivity is the 4π periodicity of the surface state spectrum. Note that the square of a glide operation is equivalent with a crystal-lattice translation. Thus, the eigenvalues of the glide operator, which is well defined on glide-invariant planes, have the form of $e^{-ik/2}$ with unusual 4π periodicity. This 4π -periodic

structure is incorporated into the surface-state dispersion of topological glide phases, and makes its shape like a Möbius strip [91, 92] (also likened to an hourglass [93]). For this reason, the surface states of topological glide superconductivity are referred to as Möbius surface states. Interestingly, topological glide superconductivity (along with topological glide insulators [92, 93, 94, 95]) is one of the rare platforms of first-order $\mathbb{Z}_4$ topological phases, which do not appear in the conventional topological periodic table of the ten Altland-Zirnbauer classes [6, 7, 8]. Such $\mathbb{Z}_4$ topological phases are a precious platform to study the interplay between topology and nonsymmorphic symmetry, and are worthy of further investigation.

1.2 Organization of this thesis

Now we can say that TSC begins to be recognized as a material phase in nature, owing to the tremendous theoretical and experimental efforts, only a part of which is presented in the previous section. Therefore, one of the important issues is to study novel topological properties of superconductivity, as well as their material proposal. This motivated us to study the following two topics presented in this thesis: material proposal of $\mathbb{Z}_4$ topological glide superconductivity and establishment of a novel bulk-boundary correspondence in one-dimensional superconductors.

The following part of this thesis is constructed as follows. First, in the remaining part of this chapter, we introduce notations related to the band theory, which are used throughout the thesis. In Chapter 2, we discuss topological properties of the paramagnetic superconducting phase of UCoGe under pressure. It is shown that the paramagnetic superconductivity is a promising candidate of $\mathbb{Z}_4$ as well as $\mathbb{Z}_2$ topological glide superconductivity. This is the first material proposal of $\mathbb{Z}_4$ topological glide superconductivity. In Chapter 3, we prove a recently proposed novel bulk-boundary correspondence in one-dimensional chiral symmetric systems. The obtained results are summarized in Chapter 4.

1.3 Notations used in this thesis

Here, we introduce the notations used throughout this thesis.

1.3.1 Real-space quantities

The creation operator of an electron at position $\mathbf{r}$ is written as $c_l^\dagger(\mathbf{r})$, with l the index for internal degrees of freedom such as spin. The position $\mathbf{r}$ is decomposed as $\mathbf{r} = \mathbf{R} + \Delta\mathbf{r}$, where $\mathbf{R}$ is the position of the unit cell and $\Delta\mathbf{r}$ is the position of the electron measured from the unit-cell center. $\Delta\mathbf{r}$ takes discrete and continuous values when tight-binding models and continuous theory are considered, respectively. Single-electron state corresponding to $c_l^\dagger(\mathbf{r})$

is written as

$$|\mathbf{r}, l\rangle = c_l^\dagger(\mathbf{r}) |\text{vac.}\rangle, \quad (1.3.1)$$

where $|\text{vac.}\rangle$ represents the vacuum state with no electrons.

We apply Seitz notation to describe space group symmetries. A space group operation g including point group operation p and translation with the displacement vector $\boldsymbol{\tau}$ is written as

$$g = \{ p \mid \boldsymbol{\tau} \}. \quad (1.3.2)$$

Accordingly, the action of g on the position $\mathbf{r}$ is given by

$$g(\mathbf{r}) = p\mathbf{r} + \boldsymbol{\tau}. \quad (1.3.3)$$

We denote the operator corresponding to g as $\hat{g}$. Its action is defined by

$$\hat{g}c_l^\dagger(\mathbf{r})\hat{g}^\dagger = c_{l'}^\dagger(p\mathbf{r} + \boldsymbol{\tau})D_{l'l}^{\text{int}}(g), \quad (1.3.4)$$

$$\hat{g}|\mathbf{r}, l\rangle = |p\mathbf{r} + \boldsymbol{\tau}, l'\rangle D_{l'l}^{\text{int}}(g), \quad (1.3.5)$$

with $D_{l'l}^{\text{int}}(g)$ the generally double-valued representation of g describing the symmetry properties of internal degrees of freedom. Here and hereafter, repeated indices are meant to be summed up.

For convenience, we define position operator for single-particle Hilbert space as follows:

$$\hat{\mathbf{r}}|\mathbf{r}, l\rangle = \mathbf{r}|\mathbf{r}, l\rangle. \quad (1.3.6)$$

When periodic boundary conditions are applied, only the form $e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}$ is well defined with $\mathbf{k}\cdot\mathbf{L} \in 2\pi\mathbb{Z}$ and $\mathbf{L}$ a diameter of the sample. However, practically speaking, bare $\hat{\mathbf{r}}$ may also be regarded as well defined when it acts on localized states such as Wannier functions. We also define the lattice point operator by

$$\hat{\mathbf{R}}|\mathbf{R} + \Delta\mathbf{r}, l\rangle = \mathbf{R}|\mathbf{R} + \Delta\mathbf{r}, l\rangle. \quad (1.3.7)$$

It is important to note that unit cell boundaries must be explicitly identified to define $\hat{\mathbf{R}}$, in contrast to $\hat{\mathbf{r}}$. When the choice of unit cells is changed, the eigenvalue of $\hat{\mathbf{R}}$ for $|\mathbf{r}, l\rangle$ is also changed. The same thing can also be said about the operator for $\Delta\mathbf{r}$:

$$\Delta\hat{\mathbf{r}}|\mathbf{R} + \Delta\mathbf{r}, l\rangle = \Delta\mathbf{r}|\mathbf{R} + \Delta\mathbf{r}, l\rangle. \quad (1.3.8)$$

$\Delta\hat{\mathbf{r}}$ is well defined regardless of boundary conditions.

For the latter use, we also discuss time-reversal symmetry. Time-reversal operator $\hat{\Theta}$ is defined to be the antiunitary operator satisfying

$$\hat{\Theta}|\mathbf{r}, l\rangle = |\mathbf{r}, l'\rangle [U_\Theta]_{l'l}. \quad (1.3.9)$$

Here, U_Θ is some unitary matrix satisfying $U_\Theta U_\Theta^* = \pm 1$. In this thesis, we consider systems with spin-orbit coupling, and therefore we set $U_\Theta U_\Theta^* = -1$ in the following. In other words, $\hat{\Theta}$ is the physical time-reversal operation rather than that combined with $SU(2)$ rotation. Since $[\hat{\Theta}, \hat{g}] = 0$,² we have

$$0 = [\hat{\Theta}, \hat{g}] |\mathbf{r}, l\rangle = |p\mathbf{r} + \boldsymbol{\tau}, l'\rangle (U_\Theta D^{\text{int}}(g)^* - D^{\text{int}}(g) U_\Theta)_{ll'}. \quad (1.3.10)$$

We obtain $\Theta D^{\text{int}}(g) \Theta^{-1} = D^{\text{int}}(g)$, where $\Theta = U_\Theta K$ and K represents complex conjugation. For example, When we consider spin as the only internal degrees of freedom (as in first-principles theory), we can identify $U_\Theta = i s_y$ with s_μ the Pauli matrix for spin. Representation matrices of symmetry operators is, for example, $D^{\text{int}}(M_x) = D^{\text{int}}(C_{2x}) = i s_x$, $D^{\text{int}}(M_y) = D^{\text{int}}(C_{2y}) = i s_y$. It can be explicitly examined that these operations commute with Θ .

1.3.2 Wave-number-space quantities

Periodic boundary conditions are often adopted to describe bulk properties. In this thesis, we consider two types of Fourier transform. The first one is the site-dependent transformation

$$c_{l, \Delta \mathbf{r}}^\dagger(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot (\mathbf{R} + \Delta \mathbf{r})} c_l^\dagger(\mathbf{R} + \Delta \mathbf{r}), \quad (1.3.11a)$$

$$|\mathbf{k}, \Delta \mathbf{r}, l\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot (\mathbf{R} + \Delta \mathbf{r})} |\mathbf{R} + \Delta \mathbf{r}, l\rangle, \quad (1.3.11b)$$

where N is the total number of unit cells. Here, $|\mathbf{k}, \Delta \mathbf{r}, l\rangle$ is an eigenstate of crystal-lattice translations:

$$\hat{T}_{\mathbf{a}} |\mathbf{k}, \Delta \mathbf{r}, l\rangle = e^{-i\mathbf{k} \cdot \mathbf{a}} |\mathbf{k}, \Delta \mathbf{r}, l\rangle, \quad (1.3.12)$$

with $\mathbf{a}$ a lattice vector and

$$\hat{T}_{\mathbf{a}} |\mathbf{R}, l\rangle = |\mathbf{R} + \mathbf{a}, l\rangle. \quad (1.3.13)$$

One of the advantages of this representation is the simpleness of the expression for space-group operations. Actually,

$$\hat{g} |\mathbf{k}, \Delta \mathbf{r}, l\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{ip\mathbf{k} \cdot (p\mathbf{R} + p\Delta \mathbf{r})} |p\mathbf{R} + p\Delta \mathbf{r} + \boldsymbol{\tau}, l'\rangle D_{ll'}^{\text{int}}(g) \quad (1.3.14a)$$

$$= e^{-ip\mathbf{k} \cdot \boldsymbol{\tau}} |p\mathbf{k}, \Delta \mathbf{r}', l'\rangle D_{\Delta \mathbf{r}' \Delta \mathbf{r}}^{\text{SL}}(g) D_{ll'}^{\text{int}}(g). \quad (1.3.14b)$$

Here, $D_{\Delta \mathbf{r}' \Delta \mathbf{r}}^{\text{SL}}(g)$ is unity for $\Delta \mathbf{r}' = g(\Delta \mathbf{r})$ modulo lattice vectors, while vanishes otherwise. $D_{\Delta \mathbf{r}' \Delta \mathbf{r}}^{\text{SL}}(g)$ represents the permutation of sublattices for the case of tight-binding models. We

² Actually, any space group operation consists of rotation, inversion, and translation. Rotation is written as $\exp(-i\boldsymbol{\theta} \cdot \hat{\mathbf{J}})$, which commutes with $\hat{\Theta}$, while inversion and translation clearly commute with $\hat{\Theta}$ as well.

write $D(g) = D^{\text{SL}}(g) \otimes D^{\text{int}}(g)$ and e.g. $\alpha = (\Delta \mathbf{r}, l)$ in the following. In particular, $D(g)$ is independent of $\mathbf{k}$. By using $U^g(\mathbf{k}) = e^{-ip\mathbf{k}\cdot\boldsymbol{\tau}} D(g)$, we obtain

$$\hat{g}c_{\alpha}^{\dagger}(\mathbf{k})\hat{g}^{\dagger} = c_{\beta}^{\dagger}(p\mathbf{k})U_{\beta\alpha}^g(\mathbf{k}), \quad (1.3.15a)$$

$$\hat{g}|\mathbf{k}, \alpha\rangle = |p\mathbf{k}, \beta\rangle U_{\beta\alpha}^g(\mathbf{k}). \quad (1.3.15b)$$

As for time-reversal symmetry, $\Theta U^g(\mathbf{k})\Theta^{-1} = U^g(-\mathbf{k})$ follows from $\Theta D^{\text{int}}(g)\Theta^{-1} = D^{\text{int}}(g)$. It should be noted that this type of Fourier transform does not have the periodicity of Brillouin zone:

$$c_{\alpha}^{\dagger}(\mathbf{k} + \mathbf{G}) = c_{\beta}^{\dagger}(\mathbf{k})V_{\beta\alpha}(\mathbf{G}), \quad (1.3.16a)$$

$$|\mathbf{k} + \mathbf{G}, \alpha\rangle = |\mathbf{k}, \beta\rangle V_{\beta\alpha}(\mathbf{G}), \quad (1.3.16b)$$

with $V_{(\Delta \mathbf{r}'l')(\Delta \mathbf{r}l)}(\mathbf{G}) = e^{i\mathbf{G}\cdot\Delta \mathbf{r}}\delta_{\Delta \mathbf{r}'\Delta \mathbf{r}}\delta_{l'l}$. Relation between $V(\mathbf{G})$ and $D(g)$ is obtained as follows:

$$V_{\beta\alpha}(\mathbf{G}) = \langle \mathbf{k}, \beta | \mathbf{k} + \mathbf{G}, \alpha \rangle \quad (1.3.17a)$$

$$= e^{-ip\mathbf{G}\cdot\boldsymbol{\tau}} D_{\beta\beta'}^{\dagger}(g) \langle p\mathbf{k}, \beta' | p(\mathbf{k} + \mathbf{G}), \alpha' \rangle D_{\alpha'\alpha}(g) \quad (1.3.17b)$$

$$= e^{-ip\mathbf{G}\cdot\boldsymbol{\tau}} [D^{\dagger}(g)V(p\mathbf{G})D(g)]_{\beta\alpha}. \quad (1.3.17c)$$

Thus, we obtain

$$V(-p\mathbf{G})D(g)V(\mathbf{G}) = e^{-ip\mathbf{G}\cdot\boldsymbol{\tau}} D(g). \quad (1.3.18)$$

The other basis for wave-number space is the one compatible with the periodicity of Brillouin zone. We define

$$c_{\mathbf{k}\alpha}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} c_l^{\dagger}(\mathbf{R} + \Delta \mathbf{r}), \quad (1.3.19a)$$

$$|\mathbf{k}, \Delta \mathbf{r}, l\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |\mathbf{R} + \Delta \mathbf{r}, l\rangle, \quad (1.3.19b)$$

It is clear that $c_{\mathbf{k}+\mathbf{G}\alpha}^{\dagger} = c_{\mathbf{k}\alpha}^{\dagger}$ and $|\mathbf{k} + \mathbf{G}, \alpha\rangle = |\mathbf{k}, \alpha\rangle$ are satisfied with $\mathbf{G}$ an arbitrary reciprocal lattice vector. In this thesis, we assign the subscript $\mathbf{k}$ to the quantities with periodic $\mathbf{k}$ dependence such as $c_{\mathbf{k},\alpha}^{\dagger}$. This basis is often used to define topological invariants, and connected to the former basis by

$$c_{\alpha}^{\dagger}(\mathbf{k}) = c_{\mathbf{k}\beta}^{\dagger} V_{\beta\alpha}(\mathbf{k}), \quad c_{\alpha}(\mathbf{k}) = V_{\alpha\beta}^{\dagger}(\mathbf{k}) c_{\mathbf{k}\beta}, \quad (1.3.20a)$$

$$|\mathbf{k}, \alpha\rangle = |\mathbf{k}, \beta\rangle V_{\beta\alpha}(\mathbf{k}). \quad (1.3.20b)$$

From these equalities, we obtain the relation of $V(\mathbf{k})$ with $\hat{\Theta}$ as follows:

$$\hat{\Theta} c_{\alpha}^{\dagger}(\mathbf{k}) \hat{\Theta}^{-1} = c_{\beta}^{\dagger}(-\mathbf{k}) [U_{\Theta}]_{\beta\alpha} = c_{\mathbf{k}\beta}^{\dagger} [V(-\mathbf{k}) U_{\Theta}]_{\beta\alpha}, \quad (1.3.21a)$$

$$\hat{\Theta} c_{\alpha}^{\dagger}(\mathbf{k}) \hat{\Theta}^{-1} = c_{-\mathbf{k}\beta}^{\dagger} [U_{\Theta} V^*(\mathbf{k})]_{\beta\alpha}. \quad (1.3.21b)$$

Thus, we obtain

$$\Theta V(\mathbf{k})\Theta^{-1} = V(-\mathbf{k}). \quad (1.3.22)$$

Note that $V(-\mathbf{k}) = V(\mathbf{k})^\dagger$ also holds by definition. For the periodic basis, we obtain

$$\hat{g}c_{\mathbf{k}\alpha}^\dagger\hat{g}^\dagger = c_{p\mathbf{k}\beta}^\dagger[U_{\mathbf{k}}^g]_{\beta\alpha}, \quad (1.3.23a)$$

$$\hat{g}|\mathbf{k}, \alpha\rangle = |p\mathbf{k}, \beta\rangle[U_{\mathbf{k}}^g]_{\beta\alpha}, \quad (1.3.23b)$$

with $U_{\mathbf{k}}^g = V(p\mathbf{k})U^g(\mathbf{k})V(\mathbf{k})^\dagger$. Clearly, $[U_{\mathbf{k}}^g]_{\beta\alpha} = (p\mathbf{k}, \beta|\hat{g}|\mathbf{k}, \alpha)$ has the periodicity of Brillouin zone: $U_{\mathbf{k}+\mathbf{G}}^g = U_{\mathbf{k}}^g$.

1.3.3 Bloch Hamiltonian and eigenstates

In this thesis, interactions are treated only at mean-field level. Therefore, Hamiltonian can be written as a bilinear of field operators by appropriately choosing the origin of energy:

$$\hat{H} = \sum_{\mathbf{r}, \mathbf{r}', l, l'} c_l^\dagger(\mathbf{r}) H_{ll'}(\mathbf{r}, \mathbf{r}') c_{l'}(\mathbf{r}'). \quad (1.3.24)$$

As long as single-particle states are concerned, $\hat{H}$ is identified with

$$\hat{H}^{(1)} = \sum_{\mathbf{r}, \mathbf{r}', l, l'} |\mathbf{r}, l\rangle H_{ll'}(\mathbf{r}, \mathbf{r}') \langle \mathbf{r}', l'|. \quad (1.3.25)$$

In Chapter 3, the symbol $\hat{H}$ is used to describe $\hat{H}^{(1)}$.

Wave-number space expressions for $\hat{H}^{(1)}$ are called Bloch Hamiltonian. In the following, we show several possible definitions and discuss their differences. The first definition is

$$\hat{H}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} \hat{H}^{(1)} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}. \quad (1.3.26)$$

This is the standard definition for continuum theory. For tight-binding models, the term “Bloch Hamiltonian” is conventionally used for Fourier transform of $H_{ll'}(\mathbf{r}, \mathbf{r}')$ denoted as $H_{\alpha\beta}(\mathbf{k}) = \langle \mathbf{k}, \alpha | \hat{H}^{(1)} | \mathbf{k}, \beta \rangle$. It follows that

$$\hat{H}^{(1)} = \sum_{\mathbf{k}, \alpha, \beta} |\mathbf{k}, \alpha\rangle H_{\alpha\beta}(\mathbf{k}) \langle \mathbf{k}, \beta|. \quad (1.3.27)$$

By using $|\mathbf{k}, \alpha\rangle = e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} |\mathbf{k} = \mathbf{0}, \alpha\rangle$, $H(\mathbf{k})$ can also be written as

$$H_{\alpha\beta}(\mathbf{k}) = \langle \mathbf{k} = \mathbf{0}, \alpha | \hat{H}(\mathbf{k}) | \mathbf{k} = \mathbf{0}, \beta \rangle. \quad (1.3.28)$$

Thus, $H(\mathbf{k})$ is the matrix element of $\hat{H}(\mathbf{k})$ with the basis independent of $\mathbf{k}$. In this sense, these two “Bloch Hamiltonians” are essentially equivalent. For example, as will be clarified below, Berry connections calculated with $\hat{H}(\mathbf{k})$ and $H(\mathbf{k})$ are equivalent with each other.

Another definition for Bloch Hamiltonian is given by

$$\hat{H}_{\mathbf{k}} = e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}} \hat{H}^{(1)} e^{i\mathbf{k}\cdot\hat{\mathbf{R}}}, \quad (H_{\mathbf{k}})_{\alpha\beta} = \langle \mathbf{k} = 0, \alpha | \hat{H}_{\mathbf{k}} | \mathbf{k} = 0, \beta \rangle. \quad (1.3.29)$$

This expression has periodicity of Brillouin zone (while $\hat{H}(\mathbf{k})$ does not), and is used to define the winding number. This is connected to the previous one by

$$\hat{H}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\Delta\hat{\mathbf{r}}} \hat{H}_{\mathbf{k}} e^{i\mathbf{k}\cdot\Delta\hat{\mathbf{r}}}, \quad H(\mathbf{k}) = V^\dagger(\mathbf{k}) H_{\mathbf{k}} V(\mathbf{k}). \quad (1.3.30)$$

Next, we discuss energy eigenstates. We define eigenstates of $\hat{H}^{(1)}$, or equivalently, single-particle energy eigenstates of $\hat{H}$, as follows:

$$\hat{H} |\psi_\mu(\mathbf{k})\rangle = \epsilon_n(\mathbf{k}) |\psi_\mu(\mathbf{k})\rangle, \quad (1.3.31)$$

which is chosen as eigenstate of translations: $\hat{T}_a |\psi_\mu(\mathbf{k})\rangle = e^{-i\mathbf{k}\cdot\mathbf{a}} |\psi_\mu(\mathbf{k})\rangle$. We require periodicity of energy eigenstates: $|\psi_\mu(\mathbf{k} + \mathbf{G})\rangle = |\psi_\mu(\mathbf{k})\rangle$ with $\mathbf{G}$ an arbitrary reciprocal lattice vector. The unit-cell-periodic part of $|\psi_\mu(\mathbf{k})\rangle$ is given by $|u_\mu(\mathbf{k})\rangle = e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} |\psi_\mu(\mathbf{k})\rangle$, and satisfies

$$\hat{H}(\mathbf{k}) |u_\mu(\mathbf{k})\rangle = \epsilon_\mu(\mathbf{k}) |u_\mu(\mathbf{k})\rangle. \quad (1.3.32)$$

Here, $|u_\mu(\mathbf{k})\rangle$ does not have the periodicity of Brillouin zone: $|u_\mu(\mathbf{k} + \mathbf{G})\rangle = e^{-i\mathbf{G}\cdot\hat{\mathbf{r}}} |u_\mu(\mathbf{k})\rangle$. It should be noticed that the space spanned by $\{|u_\mu(\mathbf{k})\rangle\}_\mu$ is equivalent to the one by $\{|\mathbf{k} = 0, \alpha\rangle\}_\alpha$, because both of them are the basis for cell-periodic states. Therefore, by using the coefficients $[\mathbf{u}_\mu(\mathbf{k})]_\alpha \equiv \langle \mathbf{k} = 0, \alpha | u_\mu(\mathbf{k}) \rangle$, we obtain an alternative description

$$H(\mathbf{k}) \mathbf{u}_\mu(\mathbf{k}) = \epsilon_\mu(\mathbf{k}) \mathbf{u}_\mu(\mathbf{k}), \quad (1.3.33)$$

which plays a central role especially for tight-binding models and superconductors. We may use either one of the descriptions to calculate, for example, Berry connection, since

$$\langle u_\mu(\mathbf{k}) | \partial_{\mathbf{k}} | u_\mu(\mathbf{k}) \rangle = \sum_{\alpha} \langle u_\mu(\mathbf{k}) | \mathbf{k} = 0, \alpha \rangle \partial_{\mathbf{k}} \langle \mathbf{k} = 0, \alpha | u_\mu(\mathbf{k}) \rangle = \mathbf{u}_\mu^\dagger(\mathbf{k}) \partial_{\mathbf{k}} \mathbf{u}_\mu(\mathbf{k}). \quad (1.3.34)$$

Similar relations hold for $\hat{H}_{\mathbf{k}}$:

$$\hat{H}_{\mathbf{k}} |u_{\mathbf{k}\mu}\rangle = \epsilon_\mu(\mathbf{k}) |u_{\mathbf{k}\mu}\rangle, \quad (1.3.35a)$$

$$H_{\mathbf{k}} \mathbf{u}_{\mathbf{k}\mu} = \epsilon_\mu(\mathbf{k}) \mathbf{u}_{\mathbf{k}\mu}, \quad (1.3.35b)$$

with $|u_{\mathbf{k}\mu}\rangle = e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}} |\psi_\mu(\mathbf{k})\rangle$ and $[\mathbf{u}_{\mathbf{k}\mu}]_\alpha = \langle \mathbf{k} = 0, \alpha | u_{\mathbf{k}\mu} \rangle$. We also obtain

$$|u_{\mathbf{k}\mu}\rangle = e^{i\mathbf{k}\cdot\Delta\hat{\mathbf{r}}} |u_\mu(\mathbf{k})\rangle, \quad (1.3.36a)$$

$$\mathbf{u}_{\mathbf{k}\mu} = V(\mathbf{k}) \mathbf{u}_\mu(\mathbf{k}). \quad (1.3.36b)$$

1.3.4 Symmetries of Bloch Hamiltonian

First, local symmetries are expressed as follows. Time-reversal symmetry of the system is given by

$$\Theta H(\mathbf{k}) \Theta^{-1} = H(-\mathbf{k}), \quad (1.3.37)$$

where $\Theta = U_\Theta K$ consists of complex conjugation K and a unitary matrix U_Θ . Particle-hole symmetry is expressed as

$$CH(\mathbf{k})C^{-1} = -H(-\mathbf{k}), \quad (1.3.38)$$

where $C = U_C K$ holds with some unitary matrix U_C . Chiral symmetry is defined by some unitary matrix Γ as

$$\Gamma H(\mathbf{k}) \Gamma^\dagger = -H(\mathbf{k}). \quad (1.3.39)$$

Symmetries for $H_{\mathbf{k}}$ are also defined by these relations.

Next, we describe crystal symmetries of normal states. Let us consider a space group symmetry $g = \{p \mid \boldsymbol{\tau}\}$ satisfying $[\hat{g}, \hat{H}] = 0$. By using $H_{\alpha\beta}(\mathbf{k}) = \langle \mathbf{k}, \alpha | \hat{H} | \mathbf{k}, \beta \rangle$ and Eq. (1.3.15b), we obtain

$$H_{\alpha\beta}(\mathbf{k}) = \langle \mathbf{k}, \alpha | \hat{g}^\dagger \hat{H} \hat{g} | \mathbf{k}, \beta \rangle = U_{\alpha'\alpha'}^g(\mathbf{k})^\dagger H_{\alpha'\beta'}(p\mathbf{k}) U_{\beta'\beta}^g(\mathbf{k}). \quad (1.3.40)$$

Thus,

$$U^g(\mathbf{k}) H(\mathbf{k}) U^g(\mathbf{k})^\dagger = H(p\mathbf{k}), \quad (1.3.41)$$

and equivalently,

$$D(g) H(\mathbf{k}) D(g)^\dagger = H(p\mathbf{k}), \quad (1.3.42)$$

hold. We also obtain

$$U_{\mathbf{k}}^g H_{\mathbf{k}} [U_{\mathbf{k}}^g]^\dagger = H_{p\mathbf{k}}. \quad (1.3.43)$$

Bloch Hamiltonian can be co-diagonalized with the symmetry operator g when $p\mathbf{k}_0 = \mathbf{k}_0 + \mathbf{G}$ holds for some reciprocal lattice vector $\mathbf{G}$. Actually, the relation $U_{\mathbf{k}_0}^g H_{\mathbf{k}_0} [U_{\mathbf{k}_0}^g]^\dagger = H_{\mathbf{k}_0}$ allows us to take Bloch states to satisfy

$$U_{\mathbf{k}_0}^g \mathbf{u}_{\mathbf{k}_0\mu}^\lambda = \lambda_{g,\mathbf{k}_0} \mathbf{u}_{\mathbf{k}_0\mu}^\lambda, \quad (1.3.44)$$

where $\lambda_{g,\mathbf{k}_0}$ is one of the eigenvalues of $U_{\mathbf{k}_0}^g$. By substituting $\mathbf{u}_{\mathbf{k}_0\mu}^\lambda = V(\mathbf{k}_0) \mathbf{u}_\mu^\lambda(\mathbf{k}_0)$, we also obtain

$$\bar{U}^g(\mathbf{k}_0) \mathbf{u}_\mu^\lambda(\mathbf{k}_0) = \lambda_{g,\mathbf{k}_0} \mathbf{u}_\mu^\lambda(\mathbf{k}_0), \quad (1.3.46)$$

with $\bar{U}^g(\mathbf{k}_0) = V^\dagger(\mathbf{k}_0) U_{\mathbf{k}_0}^g V(\mathbf{k}_0)$. Note that generally $\bar{U}^g(\mathbf{k}_0) = V(p\mathbf{k}_0 - \mathbf{k}_0) U^g(\mathbf{k}_0) \neq U^g(\mathbf{k}_0)$. The symmetry relation corresponding to $U^g(\mathbf{k}_0)$ is given by

$$U^g(\mathbf{k}_0) \mathbf{u}_\mu^\lambda(\mathbf{k}_0) = \lambda_{g,\mathbf{k}_0} \mathbf{u}_\mu^\lambda(p\mathbf{k}_0). \quad (1.3.47)$$

Chapter 2

$\mathbb{Z}_4$ topological superconductivity in UCoGe

Topological superconductivity enriched by glide symmetry, which we call ‘topological glide superconductivity’ in this thesis, is one of the most intriguing topological phases of matter: Nontrivial topology is achieved via the interplay between topology, superconductivity, and nonsymmorphic crystalline symmetries. However, to date, candidates of topological glide superconductivity are not known, except for UPt₃ as a candidate for $\mathbb{Z}_2$ topological glide superconductivity [52]. It is an urgent issue to find candidate materials for topological glide superconductivity, especially for $\mathbb{Z}_4$ topological glide superconductivity, which does not have a counterpart in conventional topological phases classified by Altrand-Zirnbauer classes.

In this chapter, we elucidate that the paramagnetic superconducting phase of UCoGe under pressure [96] is the first promising candidate of $\mathbb{Z}_4$ topological glide superconductivity. According to the *K*-theory classification, $\mathbb{Z}_4$ (and $\mathbb{Z}_2$) topological glide superconductivity may be realized in time-reversal symmetric superconductors with glide symmetry [5, 52]. In particular, odd-parity superconductivity is generally preferable to obtain non-trivial topology, as has been recognized well [2]. UCoGe is the material meeting the above conditions, for the following reasons:

1. UCoGe is considered to be a spin-triplet superconductor [53, 54]. Actually, UCoGe at ambient pressure shows the coexistence phase of ferromagnetism and superconductivity [97], suggesting equal-spin Cooper pairing. Spin-triplet superconductivity is also supported by the upper critical field extremely exceeding Pauli limit [98] as well as the almost constant Knight shift across superconducting transition [99].
2. UCoGe has paramagnetic superconducting phase under pressure [96, 100]. By applying pressure, ferromagnetism vanishes and time-reversal symmetry is recovered: Absence of internal magnetic field has been confirmed by nuclear quadrupole resonance (NQR) measurement [101]. According to the smoothness of the phase diagram [96, 100,

102, 103], the paramagnetic superconducting phase is also expected to be spin-triplet superconductivity. The huge upper critical field is also observed in this paramagnetic superconducting phase [96, 100], as well as the little change in the Knight shift [104].

3. UCoGe belongs to the space group $Pnma$ [105], which is one of the nonsymmorphic space groups and has two glide planes. This means that there are two chances to obtain nontrivial $\mathbb{Z}_4$ topological indices, which can be defined for each glide symmetry.

For these reasons, the paramagnetic superconducting phase of UCoGe under pressure is a promising candidate of time-reversal symmetric odd-parity superconductor with glide symmetries. Thus, UCoGe offers an ideal platform to study $\mathbb{Z}_4$ and $\mathbb{Z}_2$ topological glide superconductivity. We actually show that UCoGe is a promising candidate of $\mathbb{Z}_4$ as well as $\mathbb{Z}_2$ topological glide superconductivity.

This chapter is constructed as follows. The first four sections are devoted to explain technical details to obtain simplified formulas for glide topological invariants in space group $Pnma$. In Sec. 2.1, we introduce notations used in this chapter, in particular about mean-field description of superconductivity. In Sec. 2.2, we review topological invariants of time-reversal symmetric superconductivity with glide symmetry. Basic properties of $\mathbb{Z}_4$ and $\mathbb{Z}_2$ glide topological invariants are summarized for the latter use. In Sec. 2.3, we simplify the glide topological invariants by assuming additional screw symmetry which shares the axis with the glide symmetry. The topological invariants are further simplified in Sec. 2.4, by using the symmetry of $Pnma$, and are expressed by occupation number at high-symmetry points or the number of Fermi surfaces. These two sections are among the central results of this thesis. In the remaining part of the chapter, we discuss application of the formulas for glide topological invariants to the paramagnetic superconducting phase of UCoGe. In Sec. 2.5, we summarize the formulas for topological invariants obtained in the previous sections. In Sec. 2.6, the formulas are applied to the Fermi surfaces of UCoGe obtained from first-principles calculations. We make supplemental discussion on the application of our results to UCoGe in Sec. 2.7. The results obtained in this chapter is summarized in Sec. 2.8.

2.1 Notations used in this chapter

In this section, we introduce notations used in this chapter.

2.1.1 Bogoliubov-de Gennes Hamiltonian and symmetries

Here, we summarize mean-field description of superconductivity. Mean-field Hamiltonian is generally written as

$$\hat{H} = \sum_{\mathbf{k}} \phi^\dagger(\mathbf{k}) \tilde{H}_{\text{BdG}}(\mathbf{k}) \phi(\mathbf{k}), \quad (2.1.1)$$

with $\phi^\dagger(\mathbf{k}) = (\mathbf{c}^\dagger(\mathbf{k}), \mathbf{c}^T(-\mathbf{k}))$ and $[\mathbf{c}^\dagger(\mathbf{k})]_\alpha = c_\alpha^\dagger(\mathbf{k})$. $\tilde{H}_{\text{BdG}}(\mathbf{k})$ is written as

$$\tilde{H}_{\text{BdG}}(\mathbf{k}) = \begin{pmatrix} H_N(\mathbf{k}) & \tilde{\Delta}(\mathbf{k}) \\ \tilde{\Delta}(\mathbf{k})^\dagger & -H_N(-\mathbf{k})^T \end{pmatrix}_\tau. \quad (2.1.2)$$

Here, $H_N(\mathbf{k})$ is the Bloch Hamiltonian for normal state, and $\tilde{\Delta}(\mathbf{k})$ is the pair potential of superconductivity. For example, $\tilde{\Delta}(\mathbf{k}) = (\psi(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \mathbf{s})is_y$ with $\mathbf{s}$ Pauli matrices for spin, when the system has only spin degree of freedom. $\psi(\mathbf{k})$ and $\mathbf{d}(\mathbf{k})$ describe spin-singlet and -triplet components, respectively.

When the system has time-reversal symmetry $\Theta = U_\Theta K$, more convenient basis choice is given by $\Phi^\dagger(\mathbf{k}) = (\mathbf{c}^\dagger(\mathbf{k}), \mathbf{c}^T(-\mathbf{k})U_\Theta^\dagger)$. We obtain

$$\hat{H} = \sum_{\mathbf{k}} \Phi^\dagger(\mathbf{k}) H_{\text{BdG}}(\mathbf{k}) \Phi(\mathbf{k}), \quad (2.1.3)$$

$$H_{\text{BdG}}(\mathbf{k}) = \begin{pmatrix} H_N(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta(\mathbf{k})^\dagger & -H_N(\mathbf{k}) \end{pmatrix}_\tau, \quad (2.1.4)$$

with $\Delta(\mathbf{k}) = \tilde{\Delta}(\mathbf{k})U_\Theta^\dagger$. For example, $\Delta(\mathbf{k}) = \psi(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \mathbf{s}$, with time-reversal symmetry $\Theta = is_y K$. We use this basis choice in this thesis, and call $H_{\text{BdG}}(\mathbf{k})$ as Bogoliubov-de Gennes (BdG) Hamiltonian.

According to Fermi statistics, the following constraint is imposed on the pair potential:

$$\tilde{\Delta}(\mathbf{k})^T = -\tilde{\Delta}(-\mathbf{k}). \quad (2.1.5)$$

This ensures the particle-hole symmetry of $\tilde{H}_{\text{BdG}}(\mathbf{k})$ with $U_C = \tau_x$. Here, we wrote Pauli matrices for Nambu degree of freedom as τ_μ . Correspondingly, we obtain for the basis of time-reversal symmetric superconductors,

$$(\Delta(\mathbf{k})U_\Theta)^T = -\Delta(-\mathbf{k})U_\Theta, \quad (2.1.6)$$

and particle-hole symmetry with

$$U_C = \begin{pmatrix} 1 & 0 \\ 0 & U_\Theta \end{pmatrix}_\tau \tau_x \begin{pmatrix} 1 & 0 \\ 0 & U_\Theta^T \end{pmatrix}_\tau = \begin{pmatrix} 0 & U_\Theta^T \\ U_\Theta & 0 \end{pmatrix}_\tau. \quad (2.1.7)$$

For $U_\Theta = is_y$, we obtain $U_C = \tau_y s_y$. By combining Eq. (2.1.6) with time-reversal symmetry $\Theta \Delta(\mathbf{k}) \Theta^{-1} = \Delta(-\mathbf{k})$, we conclude that pair potential can be taken as an Hermitian matrix: $\Delta(\mathbf{k})^\dagger = \Delta(\mathbf{k})$. Thus, BdG Hamiltonian can be concisely written as

$$H_{\text{BdG}}(\mathbf{k}) = H_N(\mathbf{k})\tau_z + \Delta(\mathbf{k})\tau_x. \quad (2.1.8)$$

Chiral symmetry $\Gamma = \tau_y$ is evident from this expression.

Almost all the discussion in Sec. 1.3.3 holds for BdG Hamiltonian, by identifying $H(\mathbf{k})$ with $H_{\text{BdG}}(\mathbf{k})$. The only point to which attention should be paid is the treatment of crystal symmetries. Accompanied by $U(1)$ symmetry breaking, some of crystal symmetries might be broken in the superconducting phase. Let us consider a space group symmetry $g = \{ p \mid \boldsymbol{\tau} \}$ preserved in the normal state. For simplicity, we assume the point-group part of g to satisfy $p^2 = E$ as a point-group element. There are three possibilities.

1. g is preserved in the superconducting state. We call this superconducting state as g -even superconductivity. Then, BdG Hamiltonian satisfies

$$U_{\text{BdG}}^g(\mathbf{k})H_{\text{BdG}}(\mathbf{k})U_{\text{BdG}}^g(\mathbf{k})^\dagger = H_{\text{BdG}}(p\mathbf{k}), \quad (2.1.9)$$

with $U_{\text{BdG}}^g(\mathbf{k}) = U^g(\mathbf{k}) \otimes \tau_0$. In this case, by using $U_\Theta U_\Theta^* = -1$, symmetry operation satisfies

$$CU_{\text{BdG}}^g(\mathbf{k})C^{-1} = \begin{pmatrix} U_\Theta^T U_\Theta^\dagger \Theta U^g(\mathbf{k}) \Theta^{-1} U_\Theta U_\Theta^* & 0 \\ 0 & \Theta U^g(\mathbf{k}) \Theta^{-1} \end{pmatrix} = U_{\text{BdG}}^g(-\mathbf{k}). \quad (2.1.10)$$

2. g is not preserved, but the combination of g with $U(1)$ symmetry is preserved in the superconducting state. We call this state as g -odd superconductivity. BdG Hamiltonian satisfies Eq. (2.1.9) with $U_{\text{BdG}}^g(\mathbf{k}) = U^g(\mathbf{k}) \otimes \tau_z$. $U_{\text{BdG}}^g(\mathbf{k})$ anticommutes with particle-hole symmetry, $CU_{\text{BdG}}^g(\mathbf{k})C^{-1} = -U_{\text{BdG}}^g(-\mathbf{k})$.
3. Superconducting state does not have symmetries related to g . This situation may happen when superconductivity belongs to a multi-dimensional irreducible representation (or it is in the mixed-representation state). In this chapter, we consider superconductivity classified by irreducible representations of point group D_{2h} , which has only one-dimensional representations. Thus, only the cases 1 and 2 are discussed.

We also discuss the description in the Brillouin-zone periodic basis $\mathbf{c}_\mathbf{k}^\dagger$. The relation between two descriptions are given by $\Phi^\dagger(\mathbf{k}) = (\mathbf{c}_\mathbf{k}^\dagger V(\mathbf{k}), [V(-\mathbf{k})^\dagger \mathbf{c}_{-\mathbf{k}}]^T U_\Theta^\dagger) = \Phi_\mathbf{k}^\dagger V(\mathbf{k})$ (with $\otimes \tau_0$ implicit). Thus, we obtain $H_{\text{BdG},\mathbf{k}} = V(\mathbf{k})H_{\text{BdG}}(\mathbf{k})V(\mathbf{k})^\dagger$ and

$$U_{\text{BdG},\mathbf{k}}^g H_{\text{BdG},\mathbf{k}} [U_{\text{BdG},\mathbf{k}}^g]^\dagger = H_{\text{BdG},\mathbf{k}}(p\mathbf{k}), \quad (2.1.11)$$

with $U_{\text{BdG},\mathbf{k}}^g = V(p\mathbf{k})U_{\text{BdG}}^g(\mathbf{k})V(\mathbf{k})^\dagger$. We also obtain (for cases 1 and 2),

$$\Theta U_{\text{BdG},\mathbf{k}}^g \Theta^{-1} = U_{\text{BdG},-\mathbf{k}}^g, \quad CU_{\text{BdG},\mathbf{k}}^g C^{-1} = \eta_g U_{\text{BdG},-\mathbf{k}}^g, \quad (2.1.12)$$

with $\eta_g = \pm 1$ the parity of the pairing symmetry in terms of g .

2.1.2 Notations for energy eigenstates and topological invariants

In order to discuss topological properties of the system, it is convenient to define the list of occupied energy eigenstates:

$$\Psi(\mathbf{k}) = (\mathbf{u}_1(\mathbf{k}), \mathbf{u}_2(\mathbf{k}), \dots, \mathbf{u}_M(\mathbf{k})), \quad (2.1.13)$$

$$\Psi_{\mathbf{k}} = (\mathbf{u}_{k1}, \mathbf{u}_{k2}, \dots, \mathbf{u}_{kM}) = V(\mathbf{k})\Psi(\mathbf{k}), \quad (2.1.14)$$

with M the number of occupied bands. When we consider simultaneous diagonalization of Hamiltonian with some crystal symmetry $g = \{p \mid \boldsymbol{\tau}\}$, we define in a similar way

$$\Psi_{\lambda}(\mathbf{k}_0) = (\mathbf{u}_{\lambda 1}(\mathbf{k}_0), \mathbf{u}_{\lambda 2}(\mathbf{k}_0), \dots, \mathbf{u}_{\lambda M}(\mathbf{k}_0)), \quad (2.1.15a)$$

$$\Psi_{\mathbf{k}_0, \lambda} = (\mathbf{u}_{\mathbf{k}_0, \lambda 1}, \mathbf{u}_{\mathbf{k}_0, \lambda 2}, \dots, \mathbf{u}_{\mathbf{k}_0, \lambda M}) = V(\mathbf{k})\Psi_{\lambda}(\mathbf{k}_0), \quad (2.1.15b)$$

following the notations in Sec. 1.3.4. Here, $\mathbf{k}_0$ is a wave number equivalent with $p\mathbf{k}_0$ modulo a reciprocal lattice vector. It follows that

$$U_{\text{BdG}, \mathbf{k}_0}^g \Psi_{\mathbf{k}_0, \lambda} = \lambda_{g, \mathbf{k}_0} \Psi_{\mathbf{k}_0, \lambda}, \quad (2.1.16)$$

and equivalently,

$$U_{\text{BdG}}^g(\mathbf{k}_0)\Psi_{\lambda}(\mathbf{k}_0) = \lambda_{g, \mathbf{k}_0}\Psi_{\lambda}(p\mathbf{k}_0), \quad (2.1.17a)$$

$$\bar{U}_{\text{BdG}}^g(\mathbf{k}_0)\Psi_{\lambda}(\mathbf{k}_0) = \lambda_{g, \mathbf{k}_0}\Psi_{\lambda}(\mathbf{k}_0), \quad (2.1.17b)$$

with

$$\bar{U}_{\text{BdG}}^g(\mathbf{k}_0) = V(\mathbf{k}_0)^{\dagger} U_{\text{BdG}, \mathbf{k}_0}^g V(\mathbf{k}_0) = V(p\mathbf{k}_0 - \mathbf{k}_0) U_{\text{BdG}}^g(\mathbf{k}_0). \quad (2.1.18)$$

We also use similar notations when a few symmetry operators are co-diagonalized at the same time.

Topological invariants related to time-reversal symmetry is defined via Bloch functions of Kramers pairs. In this thesis, we define Kramers pair I and II by the following relation:

$$\Theta \Psi_{\mathbf{k}}^{(\text{I})} = \Psi_{-\mathbf{k}}^{(\text{II})} U_{w, -\mathbf{k}}, \quad (2.1.19a)$$

and equivalently, by $\Psi_{\mathbf{k}}^{(\text{I})} = V(\mathbf{k})\Psi^{(\text{I})}(\mathbf{k})$,

$$\Theta \Psi^{(\text{I})}(\mathbf{k}) = \Psi^{(\text{II})}(-\mathbf{k}) U_{w, -\mathbf{k}}, \quad (2.1.19b)$$

where $U_{w, \mathbf{k}}$ is a $M/2 \times M/2$ unitary matrix with M the total number of occupied bands. In particular, $U_{w, \mathbf{k}+\mathbf{G}} = U_{w, \mathbf{k}}$ for an arbitrary reciprocal lattice vector $\mathbf{G}$. We also use similar notations when we consider Kramers pair with a specific eigenvalue of some crystal symmetry.

2.2 Topology of time-reversal symmetric superconductivity with a glide plane

In this section, we review topological classification of time-reversal symmetric superconductivity with glide symmetry [5, 52]. It is well known that time-reversal symmetric superconductivity have topological invariants of class DIII. It has been shown that 2D time-reversal symmetric superconductivity with a glide symmetry has additional topological invariants protected by glide symmetry [5]: $\mathbb{Z}_4$ topological invariant θ_4 for glide-odd superconductivity and $\mathbb{Z}_2$ topological invariants $\nu_{\pm}$ for glide-even superconductivity. Here, glide-odd and -even refer to the glide parity η_G of Cooper pair, introduced in Eq. (2.1.12). We review basic properties of these topological invariants in Secs. 2.2.1, 2.2.2, and 2.2.3.

In 3D systems, we can define these 2D glide topological invariants on the two glide invariant planes in 3D Brillouin zone. Thus, topology of 3D time-reversal symmetric superconductivity with glide symmetry is specified by these glide topological invariants as well as familiar topological invariants of class DIII system. We briefly review topological classification of 3D glide-symmetric class DIII systems in Sec. 2.2.4.

2.2.1 Setup for glide topological invariants

Let us first introduce notations related to glide symmetry. Let us consider a glide symmetry G with the half-lattice translation in the $\mathbf{a}$ direction and mirror operation perpendicular to the system (i.e. parallel to $\mathbf{c}$ direction). It satisfies $G^2 = \{\bar{E}|\mathbf{a}\}$ with $\bar{E} = -E$, whose minus sign comes from 2π rotation of spin. Accordingly, we obtain

$$[U_{\text{BdG},\mathbf{k}}^G]^2 = -e^{-ik_a}. \quad (2.2.1)$$

Here, $\mathbf{k} = (k_a, k_b)$ is a two-dimensional wave number, which may be of two-dimensional system, or of a glide-invariant plane in three-dimensional Brillouin zone. Then, eigen-equation of the glide operator reads

$$U_{\text{BdG},\mathbf{k}}^G \Psi_{\mathbf{k},\pm} = \pm i e^{-ik_a/2} \Psi_{\mathbf{k},\pm}. \quad (2.2.2)$$

Glide operator satisfies the following symmetry relations with time-reversal and particle-hole symmetries:

$$\Theta U_{\text{BdG},\mathbf{k}}^G \Theta^{-1} = U_{\text{BdG},-\mathbf{k}}^G, \quad (2.2.3a)$$

$$C U_{\text{BdG},\mathbf{k}}^G C^{-1} = \eta_G U_{\text{BdG},-\mathbf{k}}^G, \quad (2.2.3b)$$

with $\eta_G = \pm 1$ the glide parity of the pairing symmetry.

An important consequence of Eq. (2.2.3) is the change of effective Altland-Zirnbauer class of glide eigensectors between $k_a = \pi$ and $k_a = 0$. On the $k_a = \pi$ line, time-reversal symmetry

is closed within each glide eigensector:

$$U_{\text{BdG},(\pi,k_b)}^G[\Theta\Psi_{(\pi,k_b),\pm}] = \pm[\Theta\Psi_{(\pi,k_b),\pm}], \quad (2.2.4)$$

while it is not at the $k_a = 0$ line:

$$U_{\text{BdG},(0,k_b)}^G[\Theta\Psi_{(0,k_b),\pm}] = \mp i[\Theta\Psi_{(0,k_b),\pm}]. \quad (2.2.5)$$

Similarly, we obtain

$$U_{\text{BdG},(\pi,k_b)}^G[C\Psi_{(\pi,k_b),\pm}] = \pm\eta_G[C\Psi_{(\pi,k_b),\pm}], \quad (2.2.6a)$$

$$U_{\text{BdG},(0,k_b)}^G[C\Psi_{(0,k_b),\pm}] = \mp i\eta_G[C\Psi_{(0,k_b),\pm}]. \quad (2.2.6b)$$

Thus, we obtain the following results:

1. For glide-even superconductivity $\eta_G = 1$, each glide eigensector at $k_a = \pi$ belongs to class DIII, while it belongs to class A at $k_a = 0$.
2. For glide-odd superconductivity $\eta_G = -1$, each glide eigensector at $k_a = \pi$ belongs to class AII, while it belongs to class D at $k_a = 0$.

These results are essential for defining glide topological invariants.

2.2.2 Glide $\mathbb{Z}_2$ topological invariant for glide-even superconductivity

We first discuss glide $\mathbb{Z}_2$ invariants, which have a conventional form. When glide-even superconductivity is considered, we can define the topological invariant of 1D class DIII systems for both positive- and negative-glide eigensectors on the $k_a = \pi$ line. Thus, $\mathbb{Z}_2$ topological invariants of glide-even superconductivity is given by [5]

$$\nu_{\pm} = \int_{-\pi}^{\pi} \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_{(\pi,k_b),\pm}^{(I)} \pmod{2}. \quad (2.2.7)$$

Here, $\boldsymbol{\beta}$ is the reciprocal lattice vector corresponding to the $\mathbf{b}$ direction, where the set $\{\mathbf{a}, \mathbf{b}\}$ ($\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$ for 3D systems) is assumed to generate all the lattice points. The Berry connection of one of the Kramers pair in the positive (negative) glide eigensector is denoted as

$$\boldsymbol{\beta} \cdot \mathbf{A}_{(\pi,k_b),\pm}^{(I)} = \text{Tr} \left[[\Psi_{(\pi,k_b),\pm}^{(I)}]^\dagger \partial_{k_b} \Psi_{(\pi,k_b),\pm}^{(I)} \right]. \quad (2.2.8)$$

It has been proposed that $\nu_{\pm}$ might be nontrivial in UPt₃ [52].

We can express $\nu_{\pm}$ in another expression where $SU(2)$ gauge invariance is explicit, following Ref. [106]. In the following, we set $\mathbf{k} = (\pi, k_b)$. From the definition of Kramers pair (2.1.19), we obtain

$$\boldsymbol{\beta} \cdot \mathbf{A}_{\mathbf{k},\pm}^{(I)} = \text{Tr} \left[[\partial_{k_b} \Theta \Psi_{\mathbf{k},\pm}^{(I)}]^\dagger \Theta \Psi_{\mathbf{k},\pm}^{(I)} \right] \quad (2.2.9a)$$

$$= \text{Tr} \left[[\partial_{k_b} \Psi_{-\mathbf{k},\pm}^{(II)} U_{w,-\mathbf{k}}]^\dagger \Psi_{-\mathbf{k},\pm}^{(II)} U_{w,-\mathbf{k}} \right] \quad (2.2.9b)$$

$$= \boldsymbol{\beta} \cdot \mathbf{A}_{-\mathbf{k},\pm}^{(II)} + \text{Tr} \left[U_{w,-\mathbf{k}}^\dagger \partial_{-k_b} U_{w,-\mathbf{k}} \right] \quad (2.2.9c)$$

$$= \boldsymbol{\beta} \cdot \mathbf{A}_{-\mathbf{k},\pm}^{(II)} + \partial_{-k_b} \log \det U_{w,-\mathbf{k}}. \quad (2.2.9d)$$

with $U_{w,\mathbf{k}}$ some unitary matrix. We used $[\Psi_{\mathbf{k},\pm}^{(II)}]^\dagger \Psi_{\mathbf{k},\pm}^{(II)} = 1$ to derive the third line. Let us introduce the matrix representation of time-reversal operator by

$$w_{\mathbf{k},\pm} = \Psi_{-\mathbf{k},\pm}^\dagger \Theta \Psi_{\mathbf{k},\pm}. \quad (2.2.10)$$

By using $\Psi_{\mathbf{k},\pm} \equiv (\Psi_{\mathbf{k},\pm}^{(I)}, \Psi_{\mathbf{k},\pm}^{(II)})$, we obtain

$$w_{\mathbf{k},\pm} = \begin{pmatrix} 0 & -U_{w,\mathbf{k}}^T \\ U_{w,-\mathbf{k}} & 0 \end{pmatrix}. \quad (2.2.11)$$

This means that $w_{\mathbf{k},\pm}$ is an antisymmetric matrix at $k_b = \Gamma_b$ for $\Gamma_b = 0, \pi$. Thus, $\text{Pf}[w_{(\pi,\Gamma_b),\pm}] = (-1)^{N_{\pm}^2/2} \det U_{w,(\pi,\Gamma_b)}$ with $N_{\pm}$ the number of occupied bands with positive (negative) glide eigenvalue. We obtain

$$\nu_{\pm} = \int_0^\pi \frac{dk_b}{\pi i} \left(\boldsymbol{\beta} \cdot \mathbf{A}_{(\pi,k_b),\pm}^{(I)} + \boldsymbol{\beta} \cdot \mathbf{A}_{(-\pi,-k_b),\pm}^{(I)} \right) \quad (2.2.12a)$$

$$= \int_0^\pi \frac{dk_b}{\pi i} \left(\boldsymbol{\beta} \cdot \mathbf{A}_{(\pi,k_b),\pm} + \partial_{k_b} \log \det U_{w,\mathbf{k}} \right) \quad (2.2.12b)$$

$$= \int_0^\pi \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_{(\pi,k_b),\pm} + \frac{1}{\pi i} \log \left[\frac{\text{Pf}[w_{(\pi,\pi)\pm}]}{\text{Pf}[w_{(\pi,0)\pm}]} \right]. \quad (2.2.12c)$$

This expression is manifestly gauge invariant under the transformation $\Psi'_{\mathbf{k},\pm} = \Psi_{\mathbf{k},\pm} U_{\chi,\mathbf{k},\pm}$ modulo two with an arbitrary unitary matrix $U_{\chi,\mathbf{k},\pm}$. This expression is used in the following sections.

When the $\mathbb{Z}_2$ invariant $\nu_{\pm}$ is nontrivial, existence of zero-energy surface states is predicted. As is usual for topological crystalline phases, the direction of the surfaces must be chosen to preserve the glide symmetry. In our case, $\mathbb{Z}_2$ surface states appear at the surface normal to $\mathbf{a} \times \mathbf{c}$.

2.2.3 Glide $\mathbb{Z}_4$ topological invariant for glide-odd superconductivity

For glide-odd superconductivity, we can define a $\mathbb{Z}_4$ topological invariant θ_4 [5]:

$$\theta_4 = 2 \int_{-\pi}^{\pi} \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_{(\pi,k_b),+}^{(I)} - \frac{1}{\pi i} \int_{0 \leq k_a \pi, -\pi \leq k_b \leq \pi} d^2 k F_{\mathbf{k},+} \pmod{4}. \quad (2.2.13)$$

Here, $F_{\mathbf{k},+}$ is the Berry curvature in the positive glide eigensector:

$$F_{\mathbf{k},+} = \epsilon_{cij} \partial_{k_i} \text{Tr} \left[\Psi_{\mathbf{k},+}^\dagger \partial_{k_j} \Psi_{\mathbf{k},+} \right], \quad (2.2.14)$$

with ϵ_{cij} the antisymmetric tensor satisfying $\epsilon_{cab} = 1$. The gauge invariance of θ_4 modulo four is clear, since the first term changes by $4\mathbb{Z}$ under gauge transformation, while the second term is gauge invariant.

Quantization of θ_4 to integer values is shown as follows. Let us consider $2\theta_4$ instead of θ_4 , since it is sufficient to show $2\theta_4 \in 2\mathbb{Z}$ for our purpose. The first term contributes to $2\theta_4$ by

$$4 \int_{-\pi}^{\pi} \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_{(\pi, k_b),+}^{(\text{I})} = 2 \int_{-\pi}^{\pi} \frac{dk_b}{\pi i} \left(\boldsymbol{\beta} \cdot \mathbf{A}_{(\pi, k_b),+}^{(\text{I})} + \boldsymbol{\beta} \cdot \mathbf{A}_{(-\pi, -k_b),+}^{(\text{I})} \right) \quad (2.2.15a)$$

$$= 2 \int_{-\pi}^{\pi} \frac{dk_b}{\pi i} \left(\boldsymbol{\beta} \cdot \mathbf{A}_{(\pi, k_b),+}^{(\text{I})} + \boldsymbol{\beta} \cdot \mathbf{A}_{(\pi, k_b),+}^{(\text{II})} \right) \pmod{4} \quad (2.2.15b)$$

$$= 2 \int_{-\pi}^{\pi} \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_{(\pi, k_b),+}. \quad (2.2.15c)$$

Therefore, by using Stokes' theorem (neglecting $4\mathbb{Z}$ contribution by gauge degree of freedom), we obtain

$$2\theta_4 = 2 \int_{-\pi}^{\pi} \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_{(0, k_b),+} \pmod{4}. \quad (2.2.16)$$

The glide eigensector on the line $k_a = 0$ effectively belongs to class D, whose topological invariant is the Berry phase. Thus, the right-hand side is quantized to $2\mathbb{Z}$, and we have established that θ_4 is a $\mathbb{Z}_4$ topological invariant.

According to the relation Eq. (2.2.16), topological properties of the states with $\theta_4 = 1, 3$ have a common feature with the Kitaev chain [1]. On the other hand, states with $\theta_4 = 2$ are totally different, and are quite interesting. However, material candidates have not been known. We will show in the subsequent sections that UCoGe is a promising candidate of $\theta_4 = 2$ topological superconductivity.

When θ_4 is nontrivial, we obtain $\mathbb{Z}_4$ surface states. As is usual for topological crystalline phases, the direction of surfaces must be chosen to preserve the glide symmetry. In this case, $\mathbb{Z}_4$ surface states appear at the surface normal to $\mathbf{a} \times \mathbf{c}$.

2.2.4 Topological classification of 3D class DIII system with glide symmetry

In this subsection, we briefly summarize the results of topological classification of 3D time-reversal symmetric superconductivity with glide symmetry, for both glide-odd and -even cases [52]. In particular, we clarify weak and strong indices of K -theory.

2.2.4.1 Topological classification of glide-odd superconductivity

Topology of time-reversal symmetric glide-odd superconductivity is specified by the three topological invariants $(W, \theta_4(0), \theta_4(\pi))$. Here, W is the three-dimensional winding number of class DIII systems, while $\theta_4(0)$ and $\theta_4(\pi)$ are 2D $\mathbb{Z}_4$ glide topological invariants defined on the two glide-invariant planes $k_c = 0, \pi$ in 3D Brillouin zone.

Due to the group structure of topological invariants, topology of an arbitrary Hamiltonian of this class can be expressed as the direct sum of the generator Hamiltonians $\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_3$, which have topological invariants shown in Table 2.1. When the topological invariants of

	W	$\theta_4(0)$	$\theta_4(\pi)$
$\mathcal{H}_1$	1	1	0
$\mathcal{H}_2$	0	0	2
$\mathcal{H}_3$	0	1	1

Table 2.1: Generators of glide-odd topological superconductivity.

the system Hamiltonian are equivalent with those of $\oplus_{i=1}^n \mathcal{H}_1 + \oplus_{i=1}^m \mathcal{H}_2 + \oplus_{i=1}^l \mathcal{H}_3$, the system is classified into the phase $(\mathbb{Z}^W, \mathbb{Z}_2^{\text{strong}}, \mathbb{Z}_4^{\text{weak}}) = (n, m, l)$. Here, $\mathbb{Z}^W$ and $\mathbb{Z}_2^{\text{strong}}$ specify strong topological indices, while $\mathbb{Z}_4^{\text{weak}}$ specifies the weak topological index. Weak (strong) topological indices mean topological indices that can (cannot) be realized by stacked 2D systems.

2.2.4.2 Topological classification of glide-even superconductivity

Topology of time-reversal symmetric glide-even superconductivity is specified by the four topological invariants $\nu_{\pm}(0), \nu_{\pm}(\pi)$. Note that winding number vanishes by even glide symmetry. Thus, topological phases are generated by $\mathcal{H}_1, \mathcal{H}_2$, and $\mathcal{H}_3$ in Table 2.2. When the

	$\nu_+(0)$	$\nu_-(0)$	$\nu_+(\pi)$	$\nu_-(\pi)$
$\mathcal{H}_1$	1	0	1	0
$\mathcal{H}_2$	0	0	1	1
$\mathcal{H}_3$	1	1	1	1

Table 2.2: Generators of glide-odd topological superconductivity.

topological invariants of Hamiltonian $\mathcal{H}$ is equivalent with those of $\oplus_{i=1}^n \mathcal{H}_1 + \oplus_{i=1}^m \mathcal{H}_2 + \oplus_{i=1}^l \mathcal{H}_3$, the system is classified into the topological phase $\{\mathbb{Z}_2^{\text{CS}_T}, \mathbb{Z}_2^{\text{strong}}, \mathbb{Z}_2^{\text{weak}}\} = \{n, m, l\}$. Here, $\mathbb{Z}_2^{\text{CS}_T}$ and $\mathbb{Z}_2^{\text{strong}}$ specify strong indices, while $\mathbb{Z}_2^{\text{weak}}$ specifies weak index.

2.3 Glide topological invariants with coaxial screw symmetry

In this section, we simplify the $\mathbb{Z}_4$ and $\mathbb{Z}_2$ glide topological invariants in the presence of coexisting screw symmetry.

2.3.1 Setup

First, we explain the setup and notations used in this section. We consider 3D time-reversal symmetric superconductivity with coaxial glide and screw symmetries. The system is assumed to be gapful in this section, and effect of nodes are discussed in Sec. 2.7. In the presence of coaxial glide and screw symmetries, we have an inversion center. We set this as the origin of a unit cell:

$$I = \{ I \mid \mathbf{0} \}. \quad (2.3.1)$$

Then, glide operation is denoted as

$$G = \{ M_c \mid \mathbf{c}/2 + \mathbf{a}/2 \}. \quad (2.3.2)$$

We set c axis to be perpendicular to the glide plane, a axis to be parallel to the direction of half-lattice translation, and b axis to be the remaining independent translation. Corresponding lattice vectors are denoted as $\mathbf{c}$, $\mathbf{a}$, and $\mathbf{b}$, respectively. The expression of screw symmetry follows as

$$S = IG = \{ C_{2c} \mid \mathbf{c}/2 + \mathbf{a}/2 \}. \quad (2.3.3)$$

As evident from this expression, the c -translation in G is necessary by the assumption of coexisting glide and screw symmetries; otherwise, IG reduces to a twofold rotation.

The wave vector is decomposed as

$$\mathbf{k} = k_a \boldsymbol{\alpha} + k_b \boldsymbol{\beta} + k_c \boldsymbol{\gamma}, \quad (2.3.4)$$

with $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\gamma}$ are the reciprocal lattice vectors corresponding to $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, respectively. For example, $\boldsymbol{\alpha}$ is given by

$$\boldsymbol{\alpha} = \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}} \quad (2.3.5)$$

and $-\pi \leq k_a \leq \pi$ holds for $\mathbf{k}$ points in the first Brillouin zone. Cyclic replacements yield $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ as well as k_b and k_c . BdG Hamiltonian is written in terms of these wave numbers: $H_{\text{BdG}}(k_a, k_b, k_c)$.

The key idea to simplify topological invariants is the relation of glide symmetry with the combined time-reversal and inversion symmetries:

$$G\Theta I = \{ E \mid \mathbf{a} + \mathbf{c} \} \Theta IG. \quad (2.3.6)$$

Accordingly, we obtain

$$|M_c \mathbf{k}, \beta\rangle [U^G(\mathbf{k})U_\Theta(U^I)^*]_{\beta\alpha} = e^{-iM_c \mathbf{k} \cdot (\mathbf{a} + \mathbf{c})} |M_c \mathbf{k}, \beta\rangle [U_\Theta(U^I U^G(\mathbf{k})^*)]_{\beta\alpha}. \quad (2.3.7)$$

Here, we used the fact that representation matrix of inversion in the $|\mathbf{k}, \alpha\rangle$ basis is independent of $\mathbf{k}$ in this case: $U^I(\mathbf{k}) = e^{-i\mathbf{k} \cdot \mathbf{0}} D(I) \equiv U^I$. Thus, we obtain

$$U_{\text{BdG}}^G(\mathbf{k})\Theta U_{\text{BdG}}^I = e^{-iM_c \mathbf{k} \cdot (\mathbf{a} + \mathbf{c})} \Theta U_{\text{BdG}}^I U_{\text{BdG}}^G(\mathbf{k}). \quad (2.3.8)$$

Let us consider glide-invariant planes specified by $k_c = \Gamma_c$ with $\Gamma_c = 0, \pi$. In the following, let us write $\mathbf{k}_c = (k_a, k_b, \Gamma_c)$. Using the notation (2.1.17b), BdG Hamiltonian is co-diagonalized with glide operator as

$$U_{\text{BdG}}^G(\mathbf{k}_c)\Psi_\pm(\mathbf{k}_c) = \pm i e^{-ik_a/2} \Psi_\pm(M_c \mathbf{k}_c). \quad (2.3.9)$$

From Eq. (2.3.8), we obtain

$$U_{\text{BdG}}^G(\mathbf{k}_c)[\Theta U_{\text{BdG}}^I \Psi_\pm(\mathbf{k}_c)] = e^{-iM_c \mathbf{k}_c \cdot (\mathbf{a} + \mathbf{c})} (\mp i e^{ik_a/2}) [\Theta U_{\text{BdG}}^I \Psi_\pm(M_c \mathbf{k}_c)]. \quad (2.3.10)$$

Note that $\mathbf{G}_c \equiv M_c \mathbf{k}_c - \mathbf{k}_c = (0, 0, 2\Gamma_c)$ is a reciprocal lattice vector. This leads to the identity

$$\Theta U_{\text{BdG}}^I V(\mathbf{G}_c) = V(\mathbf{G}_c) \Theta U_{\text{BdG}}^I, \quad (2.3.11)$$

from Eq. (1.3.22) and (1.3.18). Thus, we obtain

$$\bar{U}_{\text{BdG}}^G(\mathbf{k}_c)\Psi_\pm(\mathbf{k}_c) = \pm i e^{-ik_a/2} \Psi_\pm(\mathbf{k}_c), \quad (2.3.12a)$$

$$\bar{U}_{\text{BdG}}^G(\mathbf{k}_c)[\Theta U_{\text{BdG}}^I \Psi_\pm(\mathbf{k}_c)] = \pm i e^{-ik_a/2} [\Theta U_{\text{BdG}}^I \Psi_\pm(\mathbf{k}_c)], \quad (2.3.12b)$$

for $\Gamma_c = \pi$. This means that time-reversal inversion closes within each glide-eigensector for $\Gamma_c = \pi$, allowing us to simplify topological invariants. We discuss details in the following subsections.

2.3.2 $\mathbb{Z}_4$ topological invariant in the presence of screw symmetry

2.3.2.1 Simplification of $\mathbb{Z}_4$ invariant by eigenvalues of Bogoliubov quasiparticles

Let us discuss simplification of the $\mathbb{Z}_4$ topological invariant. For convenience, we use the basis of site-dependent Fourier transform (Eq. (2.1.13)) in this section. Let us first rewrite the $\mathbb{Z}_4$ invariant (2.2.13) in this basis. For this purpose, we make a discussion parallel to Sec. 2.2.2 and then substitute $\Psi_{\mathbf{k}+} = \Psi_+(\mathbf{k})V(\mathbf{k})$, to obtain

$$\theta_4(\pi) = 2 \int_0^\pi \frac{dk_b}{\pi i} \beta \cdot \mathbf{A}_{(\pi, k_b, \pi)+} + \frac{2}{\pi i} \log \left[\frac{\text{Pf}[w_{\Gamma_2, +}]}{\text{Pf}[w_{\Gamma_1, +}]} \right] - \frac{1}{\pi i} \int_{0 \leq k_a \leq \pi} d^2 k F_{\mathbf{k}_c, +} \quad (2.3.13a)$$

$$= 2 \int_0^\pi \frac{dk_b}{\pi i} \beta \cdot \mathbf{A}_+(\pi, k_b, \pi) + \frac{2}{\pi i} \log \left[\frac{\text{Pf}[w_+(\Gamma_2)]}{\text{Pf}[w_+(\Gamma_1)]} \right] - \frac{1}{\pi i} \int_{0 \leq k_a \leq \pi} d^2 k F_+(\mathbf{k}_c) + \delta\theta_4. \quad (2.3.13b)$$

We denoted $\mathbb{Z}_4$ invariant as $\theta_4(\pi)$ to stress $k_c = \pi$ is considered. Here, Γ_1 and Γ_2 are given by $(\pi, 0, \pi)$ and (π, π, π) , respectively. There is a correction term between two basis denoted as $\delta\theta_4$, given by

$$\delta\theta_4 = 2 \int_0^\pi \frac{dk_b}{\pi} \boldsymbol{\beta} \cdot \mathbf{r}_{(\pi, k_b, \pi)+}^{\text{occ.}} - \frac{1}{\pi} \int_{0 \leq k_a \leq \pi} d^2 k \hat{c} \cdot \nabla_{\mathbf{k}} \times \mathbf{r}_{\mathbf{k}_c+}^{\text{occ.}}, \quad (2.3.14a)$$

$$i\mathbf{r}_{\mathbf{k}_+}^{\text{occ.}} = \text{Tr} [\Psi_+(\mathbf{k}) \Psi_+^\dagger(\mathbf{k}) V(\mathbf{k})^\dagger \partial_{\mathbf{k}} V(\mathbf{k})] = \text{Tr} [P_{\mathbf{k}_+}^{\text{occ.}} [\partial_{\mathbf{k}} V(\mathbf{k})] V(\mathbf{k})^\dagger], \quad (2.3.14b)$$

with $P_{\mathbf{k}_+}^{\text{occ.}} = \Psi_{\mathbf{k}_+} \Psi_{\mathbf{k}_+}^\dagger$ the projection operator onto occupied states with positive glide eigenvalue. Note that the second term in Eq. (2.3.13a) is invariant under change of the basis, since

$$w_{\mathbf{k}_+} = \Psi_+(-\mathbf{k})^\dagger V(-\mathbf{k})^\dagger \Theta V(\mathbf{k}) \Psi_+(\mathbf{k}) = w_+(\mathbf{k}). \quad (2.3.15)$$

It can be shown that $\delta\theta_4$ is the effect purely from atomic positions within unit cells, and is a constant independent of, in particular, chemical potential. In order to see this, let us focus on the $k_a = \pi$ line. Time-reversal symmetry imposes the constraint $\Theta P_{(\pi, k_b, \pi)+}^{\text{occ.}} \Theta^{-1} = P_{(\pi, -k_b, \pi)+}^{\text{occ.}}$ ¹ which leads to $\mathbf{r}_{(\pi, k_b, \pi)+}^{\text{occ.}} = \mathbf{r}_{(\pi, -k_b, \pi)+}^{\text{occ.}}$. By using Stokes' theorem with the fact that $\mathbf{r}_{\mathbf{k}_+}^{\text{occ.}}$ is gauge invariant, we obtain

$$\delta\theta_4 = \int_{-\pi}^\pi \frac{dk_b}{\pi} \boldsymbol{\beta} \cdot \mathbf{r}_{(0, k_b, \pi)+}^{\text{occ.}}. \quad (2.3.17)$$

Owing to particle-hole symmetry at $k_a = 0$, the constraint $C P_{(0, k_b, \pi)+}^{\text{occ.}} C^{-1} = P_{(0, -k_b, \pi)+}^{\text{unocc.}}$ is obtained with $P_{\mathbf{k}_+}^{\text{unocc.}}$ the projection operator onto unoccupied states with positive glide eigenvalue. Projection operator onto positive glide eigenspace is given by $P_{\mathbf{k}_+} = P_{\mathbf{k}_+}^{\text{occ.}} + P_{\mathbf{k}_+}^{\text{unocc.}}$ and satisfies $\Theta P_{(0, k_b, \pi)+} \Theta^{-1} = P_{(0, -k_b, \pi)-}$. Therefore, $\delta\theta_4$ is rewritten as

$$\delta\theta_4 = \int_{-\pi}^\pi \frac{dk_b}{4\pi i} \text{Tr} [[\partial_{k_b} V(0, k_b, 0)] V(0, k_b, 0)^\dagger]. \quad (2.3.18a)$$

Thus, $\delta\theta_4$ is determined only from atomic positions and choice of unit cells.

From the expression of $\mathbb{Z}_4$ invariant (2.2.13), $\theta_4(\pi) = 0$ at $\mu \rightarrow -\infty$, where BdG Hamiltonian is $\mathbf{k}$ independent. Thus, $\mathbb{Z}_4$ invariant $\theta_4(\pi)$ can be obtained from $\theta_4(\pi) = \theta_4(\pi) - \theta_4(\pi)|_{\mu \rightarrow -\infty}$, and thus, from the difference of the first three terms in Eq. (2.3.13) rather than a direct evaluation of $\delta\theta_4$.² In the following, we concentrate on the first three terms of Eq. (2.3.13).

¹ This follows from the following identity. For arbitrary states ϕ and ψ , $P = \mathbf{u}\mathbf{u}^\dagger$ satisfies

$$\phi^\dagger (\Theta P \Theta^{-1} \psi) = (P \Theta^{-1} \psi)^\dagger \Theta^{-1} \phi = (\Theta^{-1} \psi)^\dagger \mathbf{u}\mathbf{u}^\dagger \Theta^{-1} \phi = \phi^\dagger [\Theta \mathbf{u} (\Theta \mathbf{u})^\dagger] \psi. \quad (2.3.16)$$

²In Ref. [3], we have directly evaluated $\theta_4(\pi)$, and have shown that $\delta\theta_4$ is an integer related to the character of representation matrix of inversion.

An important consequence of ΘI symmetry is $F_+(\mathbf{k}_c) = 0$. This is proven as follows:

$$F_+(\mathbf{k}_c) = \epsilon_{cij} \partial_{k_i} \text{Tr} [\Psi_+(\mathbf{k}_c)^\dagger \partial_{k_j} \Psi_+(\mathbf{k}_c)] \quad (2.3.19a)$$

$$= \epsilon_{cij} \partial_{k_i} \text{Tr} [\partial_{k_j} \Theta U_{\text{BdG}}^I \Psi_+(\mathbf{k}_c)^\dagger \Theta U_{\text{BdG}}^I \Psi_+(\mathbf{k}_c)] \quad (2.3.19b)$$

$$= \epsilon_{cij} \partial_{k_i} \text{Tr} [\partial_{k_j} \Psi_+(\mathbf{k}_c) v_+(\mathbf{k}_c)^\dagger \Psi_+(\mathbf{k}_c) v_+(\mathbf{k}_c)] \quad (2.3.19c)$$

$$= -F_+(\mathbf{k}_c) - \epsilon_{cij} \partial_{k_i} \partial_{k_j} \log \det v_+(\mathbf{k}_c) \quad (2.3.19d)$$

$$= -F_+(\mathbf{k}_c), \quad (2.3.19e)$$

where we introduced

$$v_+(\mathbf{k}_c) = \Psi_+^\dagger(\mathbf{k}_c) \Theta U_{\text{BdG}}^I \Psi_+(\mathbf{k}_c). \quad (2.3.20)$$

This is an antisymmetric unitary matrix: $v_+(\mathbf{k}_c) = -v_+^T(\mathbf{k}_c)$, $v_+(\mathbf{k}) v_+(\mathbf{k})^\dagger = 1$, and is related to $w_+(\mathbf{k}_c)$ by

$$v_+(\mathbf{k}_c) = \Psi_+^\dagger(\mathbf{k}_c) U_{\text{BdG}}^I \Psi_+(-\mathbf{k}_c) w_+(\mathbf{k}_c). \quad (2.3.21)$$

Now we have only to consider $k_a = \pi$ line to evaluate $\theta_4(\pi) - \delta\theta_4$:

$$\theta_4(\pi) - \delta\theta_4 = 2 \int_0^\pi \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_+(\pi, k_b, \pi) + \frac{2}{\pi i} \log \left[\frac{\text{Pf}[w_+(\Gamma_2)]}{\text{Pf}[w_+(\Gamma_1)]} \right]. \quad (2.3.22)$$

It should be noted that inversion symmetry closes within each glide eigensector on this line. Thus, each glide eigensector can be regarded as class AII insulator with inversion symmetry. This fact enables us to follow the discussion of the Fu-Kane criteria for inversion symmetric topological insulators [107], to simplify $\theta_4(\pi) - \delta\theta_4$.

One of the essential ideas of Ref. [107] is to introduce the so-called transverse gauge, where $A_+(k)$ identically vanishes (in the following, we write $k = (0, k_b, \pi)$). In order to see such a gauge choice is possible, let us focus on

$$A_+(k) = -\frac{1}{2} \partial_{k_b} \log \text{Pf}[v_+(k)], \quad (2.3.23)$$

which is obtained following the discussion of $F_+(\mathbf{k}_c)$ with $\det[v_+(k)] = \text{Pf}[v_+(k)]^2$. It means that $A_+(k)$ vanishes if we can choose a gauge such that $\text{Pf}[v_+(k)] \equiv 1$. Indeed, such a gauge is obtained by a gauge transformation

$$\Psi_+(k) \rightarrow \Psi_+(k) U_{\text{tr},k}, \quad (2.3.24a)$$

$$\text{Pf}[v_+(k)] \rightarrow \text{Pf}[U_{\text{tr},k}^\dagger v_+(k) U_{\text{tr},k}^*] = \text{Pf}[v_+(k)] \det U_{\text{tr},k}^*, \quad (2.3.24b)$$

with $\det U_{\text{tr}} = \text{Pf}[v_+(k)] / |\text{Pf}[v_+(k)]|$. For example, we can just retake the phase of one of the Bloch states as $\mathbf{u}_+(k) \rightarrow (\text{Pf}[v_+(k)] / |\text{Pf}[v_+(k)]|) \mathbf{u}_+(k)$ to obtain $U_{\text{tr},k}$.

In the transverse gauge, $w_+(\Gamma_i)$ ($i = 1, 2$) is easily calculated. Let us retake basis of Kramers degree of freedom as the eigenstate of inversion at Γ_i , ($i = 1, 2$):

$$\bar{U}_{\text{BdG}}^I(\Gamma_i) \Psi_+^{(1)}(\Gamma_i) = \Psi_+^{(1)}(\Gamma_i) \xi_{\text{BdG}}(\Gamma_i), \quad (2.3.25)$$

with $\xi_{\text{BdG}}(\Gamma_i)$ a diagonal matrix whose components are ± 1 , and

$$\bar{U}_{\text{BdG}}^I(\Gamma_i) = V(2\Gamma_i)U_{\text{BdG}}^I = V^\dagger(\Gamma_i)U_{\text{BdG},\Gamma_i}^I V(\Gamma_i), \quad (2.3.26)$$

which squares to unity (see Eq. (2.1.18)). The above discussion remains valid in this basis, since we did not use special properties of $\Psi_+^{(\text{I})}(\mathbf{k})$ (in particular, transverse gauge can be taken within this basis choice).

The matrix element of inversion operator is evaluated as follows:

$$\Psi_+(\Gamma_i)^\dagger U_{\text{BdG}}^I \Psi_+(-\Gamma_i) = \Psi_+(\Gamma_i)^\dagger [\bar{U}_{\text{BdG}}^I(\Gamma_i)]^\dagger \Psi_+(\Gamma_i) \quad (2.3.27a)$$

$$= \begin{pmatrix} \Psi_+^{(\text{I})}(\Gamma_i)^\dagger \bar{U}_{\text{BdG}}^I \Psi_+^{(\text{I})}(\Gamma_i) & 0 \\ 0 & \Psi_+^{(\text{II})}(\Gamma_i)^\dagger \bar{U}_{\text{BdG}}^I \Psi_+^{(\text{II})}(\Gamma_i) \end{pmatrix} \quad (2.3.27b)$$

$$= \begin{pmatrix} \xi_{\text{BdG}}(\Gamma_i) & 0 \\ 0 & U_{w,\Gamma_i} \xi_{\text{BdG}}(\Gamma_i) U_{w,\Gamma_i}^\dagger \end{pmatrix}, \quad (2.3.27c)$$

(see Eq. (2.2.11)). Therefore, from Eq. (2.3.21), the matrix $v_+(\Gamma_i)$ is given by

$$v_+(\Gamma_i) = \begin{pmatrix} \xi_{\text{BdG}}(\Gamma_i) & 0 \\ 0 & U_{w,\Gamma_i} \xi_{\text{BdG}}(\Gamma_i) U_{w,\Gamma_i}^\dagger \end{pmatrix} \begin{pmatrix} 0 & -U_{w,\Gamma_i}^T \\ U_{w,\Gamma_i} & 0 \end{pmatrix} \quad (2.3.28a)$$

$$= \begin{pmatrix} 0 & -\xi_{\text{BdG}}(\Gamma_i) U_{w,\Gamma_i}^T \\ U_{w,\Gamma_i} \xi_{\text{BdG}}(\Gamma_i) & 0 \end{pmatrix}, \quad (2.3.28b)$$

leading to $\text{Pf}[v_+(\Gamma_i)] = (-1)^{N_+^2/2} \det U_{w,\Gamma_i} \det \xi_{\text{BdG}}(\Gamma_i) = \text{Pf}[w_+(\Gamma_i)] \det \xi_{\text{BdG}}(\Gamma_i)$. Since $\text{Pf}[v_+(\Gamma_i)] = 1$, we obtain $\text{Pf}[w_+(\Gamma_i)] = \det \xi_{\text{BdG}}(\Gamma_i) = \pm 1$. Finally, we obtain

$$\theta_4(\pi) - \delta\theta_4 = \frac{2}{\pi i} \log \left[\frac{\det \xi_{\text{BdG}}(\Gamma_2)}{\det \xi_{\text{BdG}}(\Gamma_1)} \right], \quad (2.3.29)$$

and equivalently,

$$(-1)^{(\theta_4(\pi) - \delta\theta_4)/2} = \det \xi_{\text{BdG}}(\Gamma_2) \det \xi_{\text{BdG}}(\Gamma_1). \quad (2.3.30)$$

2.3.2.2 Simplification of $\mathbb{Z}_4$ invariant by the eigenvalues of electrons

Next, we reduce $\det \xi_{\text{BdG}}(\Gamma_i)$ to the inversion eigenvalues of the occupied normal state. This is achieved via the so-called weak pairing assumption, following Ref. [57, 108]. Except for accidental cases, Fermi surfaces are off Γ_i , and therefore, we can adiabatically vanish order parameter without closing the gap at Γ_i . This is always possible when order parameter is sufficiently smaller than the Fermi energy, and is considered to be satisfied for most cases.

Note that the eigen-equation

$$\bar{U}_{\text{BdG}}^I(\Gamma_i) \Psi_+^{(\text{I})}(\Gamma_i) = \Psi_+^{(\text{I})}(\Gamma_i) \xi_{\text{BdG}}(\Gamma_i) \quad (2.3.31)$$

is rewritten as

$$U_{\text{BdG},\Gamma_i}^I \Psi_{\Gamma_i,+}^{(I)} = \Psi_{\Gamma_i,+}^{(I)} \xi_{\text{BdG}}(\Gamma_i). \quad (2.3.32)$$

In the following, we use the basis of $\Psi_{\Gamma_i,+}$ instead of $\Psi_+(\Gamma_i)$ for convenience. In the weak-pairing limit, BdG Hamiltonian is given by

$$H_{\text{BdG},\Gamma_i} = H_{N,\Gamma_i} \tau_z + (+0) \Delta_{\Gamma_i} \tau_x. \quad (2.3.33)$$

We leave the infinitesimal order parameter, to remind us of the constraint between particle-hole and inversion symmetries:

$$CU_{\text{BdG},\Gamma_i}^I = \eta_I U_{\text{BdG},\Gamma_i}^I C, \quad (2.3.34a)$$

$$CU_{\text{BdG},\Gamma_i}^G = \eta_G U_{\text{BdG},\Gamma_i}^G C, \quad (2.3.34b)$$

with $\eta_I = \pm 1$ and $\eta_G = -1$ the inversion-parity of the pairing symmetry (we leave $\eta_G = -1$ implicit for the latter convenience). Let us co-diagonalize $H_N(\Gamma_i)$ with normal-state representation matrices of glide and inversion. The list of one of the Kramers pair satisfies

$$U_{\Gamma_i}^G \phi_{\Gamma_i,\pm,(\text{un})\text{occ.}}^{(I)} = \pm \phi_{\Gamma_i,\pm,(\text{un})\text{occ.}}^{(I)}, \quad (2.3.35a)$$

$$U_{\Gamma_i}^I \phi_{\Gamma_i,\pm,(\text{un})\text{occ.}}^{(I)} = \phi_{\Gamma_i,\pm,(\text{un})\text{occ.}}^{(I)} \xi_{\pm,(\text{un})\text{occ.}}(\Gamma_i), \quad (2.3.35b)$$

with $\xi_{\pm,(\text{un})\text{occ.}}(\Gamma_i)$ a diagonal matrix whose components are ± 1 . Here, the subscript (un)occ. means (un)occupied state of $H_N(\Gamma_i)$. By using this, we can constitute $\Psi_{\Gamma_i,+}^{(I)}$ as follows:

$$\Psi_{\Gamma_i,+}^{(I)} = \left(\begin{pmatrix} \phi_{\Gamma_i,+,\text{occ.}}^{(I)} \\ 0 \end{pmatrix}_\tau, C \begin{pmatrix} \phi_{\Gamma_i,\eta_G,\text{unocc.}}^{(I)} \\ 0 \end{pmatrix}_\tau \right). \quad (2.3.36)$$

It is easily examined that $U_{\text{BdG}}^G \Psi_{\Gamma_i,+}^{(I)} = \Psi_{\Gamma_i,+}^{(I)}$ is satisfied and $\Psi_{\Gamma_i,+}^{(I)}$ is the list of eigenstates with negative eigenvalues of H_{BdG,Γ_i} , by using Eq. (2.3.34) and $U_{\text{BdG},\Gamma_i}^G = U_{\Gamma_i}^G \otimes \text{diag}(1, \eta_G)_\tau$. We obtain

$$U_{\text{BdG},\Gamma_i}^I \Psi_{\Gamma_i,+}^{(I)} = \Psi_{\Gamma_i,+}^{(I)} \begin{pmatrix} \xi_{+,\text{occ.}}(\Gamma_i) & 0 \\ 0 & \eta_I \xi_{\eta_G,\text{unocc.}}(\Gamma_i) \end{pmatrix} \quad (2.3.37)$$

and accordingly, $\det \xi_{\text{BdG}}(\Gamma_i) = \det \xi_{+,\text{occ.}}(\Gamma_i) \det \eta_I \xi_{\eta_G,\text{unocc.}}(\Gamma_i)$. Thus, we obtain

$$(-1)^{(\theta_4(\pi) - \delta\theta_4)/2} = \prod_{i=1,2} \det \xi_{+,\text{occ.}}(\Gamma_i) \det \eta_I \xi_{\eta_G,\text{unocc.}}(\Gamma_i). \quad (2.3.38)$$

In order to go further, let us introduce number of occupied electron states with glide and inversion eigenvalues. Let us define $2N_{\pm,g}(\Gamma_i)$ as the number of occupied normal states at Γ_i with positive (negative) glide and positive inversion eigenvalues. The factor 2 comes from Kramers degeneracy. In the same way, we define $2N_{\pm,u}(\Gamma_i)$ as the number of occupied normal states at Γ_i with positive (negative) glide and negative inversion eigenvalues. We also define

$N_{\pm}(\Gamma_i) = N_{\pm,g}(\Gamma_i) + N_{\pm,u}(\Gamma_i)$ and $N_{g(u)}(\Gamma_i) = N_{+,g(u)}(\Gamma_i) + N_{-,g(u)}(\Gamma_i)$. Furthermore, we add superscript “occ.” and “unocc.” to specify occupied and unoccupied states, respectively, while add “tot.” to their summation. Based on this notation, we obtain

$$(-1)^{(\theta_4(\pi) - \delta\theta_4)/2} = \prod_{i=1,2} (-1)^{N_{+,u}^{\text{occ.}}(\Gamma_i)} (-1)^{N_{\eta_G, u}^{\text{unocc.}}(\Gamma_i)} \eta_I^{N_{\eta_G}^{\text{unocc.}}(\Gamma_i)} \quad (2.3.39a)$$

$$= \prod_{i=1,2} (-1)^{N_{+,u}^{\text{occ.}}(\Gamma_i)} (-1)^{N_{\eta_G, -\eta_I}^{\text{unocc.}}(\Gamma_i)} \quad (2.3.39b)$$

$$= \left(\prod_{i=1,2} (-1)^{N_{\eta_G, -\eta_I}^{\text{tot.}}(\Gamma_i)} \right) \prod_{i=1,2} (-1)^{N_{+,u}^{\text{occ.}}(\Gamma_i)} (-1)^{N_{\eta_G, -\eta_I}^{\text{occ.}}(\Gamma_i)}, \quad (2.3.39c)$$

where $\eta_I = +1(-1)$ corresponds to $g(u)$. On the other hand, we obtain

$$(-1)^{(\theta_4(\pi) - \delta\theta_4)/2} \big|_{\mu \rightarrow -\infty} = \left(\prod_{i=1,2} (-1)^{N_{\eta_G, -\eta_I}^{\text{tot.}}(\Gamma_i)} \right). \quad (2.3.40)$$

Thus, we conclude from $\theta_4(\pi) = (\theta_4(\pi) - \delta\theta_4) - (\theta_4(\pi) - \delta\theta_4) \big|_{\mu \rightarrow -\infty}$,

$$\theta_4(\pi)/2 = \sum_{i=1,2} N_{+,u}^{\text{occ.}}(\Gamma_i) + N_{\eta_G, -\eta_I}^{\text{occ.}}(\Gamma_i) \pmod{2} \quad (2.3.41a)$$

$$= \sum_{i=1,2} N_{+,u}^{\text{occ.}}(\Gamma_i) + N_{-, -\eta_I}^{\text{occ.}}(\Gamma_i) \pmod{2}. \quad (2.3.41b)$$

2.3.3 $\mathbb{Z}_2$ topological invariants in the presence of screw symmetry

We can derive a similar formula for $\mathbb{Z}_2$ topological invariant. Let us first rewrite $\nu_{\pm}(\pi)$ in the basis of $\Psi_{\pm}(\mathbf{k}_c)$:

$$\nu_{\pm}(\pi) = \int_0^{\pi} \frac{dk_b}{\pi i} \boldsymbol{\beta} \cdot \mathbf{A}_{\pm}(\pi, k_b, \pi) + \frac{1}{\pi i} \log \left[\frac{\text{Pf}[w_{\pm}(\Gamma_2)]}{\text{Pf}[w_{\pm}(\Gamma_1)]} \right] + \delta\nu_{\pm}, \quad (2.3.42)$$

with

$$\delta\nu_{\pm} = \int_0^{\pi} \frac{dk_b}{\pi} \boldsymbol{\beta} \cdot \mathbf{r}_{(\pi, k_b, \pi)\pm}^{\text{occ.}}. \quad (2.3.43)$$

Here, time-reversal symmetry and chiral symmetry, which close on $k_a = \pi$ line, ensure that

$$\delta\nu_{\pm} = \int_{-\pi}^{\pi} \frac{dk_b}{4\pi} \boldsymbol{\beta} \cdot (\mathbf{r}_{(\pi, k_b, \pi)\pm}^{\text{occ.}} + \mathbf{r}_{(\pi, k_b, \pi)\pm}^{\text{unocc.}}) \quad (2.3.44a)$$

$$= \int_{-\pi}^{\pi} \frac{dk_b}{4\pi i} \text{Tr} \left[P_{(\pi, k_b, \pi)\pm} [\partial_{k_b} V(\pi, k_b, \pi)] V(\pi, k_b, \pi)^{\dagger} \right]. \quad (2.3.44b)$$

$\delta\nu_{\pm}$ is independent of μ , as is $\delta\theta_4$, since $P_{(\pi, k_b, \pi)\pm} = (1 \pm U_{\text{BdG}, (\pi, k_b, \pi)}^G)/2$.³ Thus, we can make a discussion parallel to $\theta_4(\pi)$ to simplify $\nu_{\pm}$, since $2(\nu_{+} - \delta\nu_{+})$ has exactly the same

³It can be easily shown by an explicit calculation that $2\delta\nu_{\pm} = \delta\theta_4$, by using $V(\mathbf{k}) = e^{i\mathbf{k} \cdot \Delta \mathbf{r}}$ and $\text{Tr}[U_{\text{BdG}, \mathbf{k}}^G] \propto \text{Tr}[s_c] = 0$ with s_c the Pauli matrix of the Kramers degree of freedom.

form as Eq. (2.3.22). Finally, we obtain

$$\nu_{\pm} = \sum_{i=1,2} N_{\pm,u}^{\text{occ.}}(\Gamma_i) + N_{\pm\eta_G, -\eta_I}^{\text{occ.}}(\Gamma_i) \pmod{2} \quad (2.3.45a)$$

$$= \sum_{i=1,2} N_{\pm,u}^{\text{occ.}}(\Gamma_i) + N_{\pm, -\eta_I}^{\text{occ.}}(\Gamma_i) \pmod{2}, \quad (2.3.45b)$$

with $\eta_G = +1$. In particular, $\nu = \sum_{i=1,2} 2N_{\pm,u}^{\text{occ.}}(\Gamma_i) = 0$ modulo 2 for even-parity superconductivity $\eta_I = +1$. For odd-parity superconductivity $\eta_I = -1$,

$$\nu_{\pm} = \sum_{i=1,2} N_{\pm}^{\text{occ.}}(\Gamma_i), \pmod{2}. \quad (2.3.46)$$

This result is consistent with the fact that topological invariants of class DIII odd-parity superconductors are determined by the number of Fermi surfaces [57, 108, 109].

2.4 Formulas for glide topological invariants in space group $Pnma$

In this section, we take advantage of symmetries of $Pnma$ to further simplify topological invariants. Space group $Pnma$ consists of inversion, two glide, mirror, and three screw symmetries, along with translations. Below, we write down a representative form of each element:

$$E = \{ E \mid \mathbf{0} \}, \quad I = \{ I \mid \mathbf{0} \}, \quad (2.4.1a)$$

$$G_z = \{ M_z \mid (\hat{x} + \hat{z})/2 \}, \quad M_y = \{ M_y \mid \hat{y}/2 \}, \quad G_x = \{ M_x \mid (\hat{x} + \hat{y} + \hat{z})/2 \}, \quad (2.4.1b)$$

$$S_z = \{ C_{2z} \mid (\hat{x} + \hat{z})/2 \}, \quad S_y = \{ C_{2y} \mid \hat{y}/2 \}, \quad S_x = \{ C_{2x} \mid (\hat{x} + \hat{y} + \hat{z})/2 \}. \quad (2.4.1c)$$

For the latter use, we summarize some of the relations between space group operations:

$$G_z I = \{ E \mid \hat{x} + \hat{z} \} G_z I, \quad G_z M_y = -M_y G_z, \quad M_y I = \{ E \mid \hat{y} \} I M_y, \quad (2.4.2)$$

$$G_x I = \{ E \mid \hat{x} + \hat{y} + \hat{z} \} I G_x, \quad M_y G_x = -\{ E \mid -\hat{y} \} G_x M_y, \quad (2.4.3)$$

where we introduced $-1 = \bar{E}$ to describe 2π rotation of spin.

Since there are two glide planes, we can define two glide topological invariants corresponding to G_z and G_x . We consider each glide symmetry separately, in the following.

2.4.1 Topological invariants by G_z

We first consider topological invariants ensured by $G_z = \{ M_z \mid (\hat{x} + \hat{z})/2 \}$. In this case, we can use the discussion of Sec. 2.3 by setting $\mathbf{a} = \hat{x}$, $\mathbf{b} = \hat{y}$, and $\mathbf{c} = \hat{z}$. Thus, we obtain $k_a = k_x$, $k_b = k_y$, and $k_c = k_z$, leading to

$$\Gamma_1 : U = (k_x = \pi, k_y = 0, k_z = \pi), \quad \Gamma_2 : R = (k_x = \pi, k_y = \pi, k_z = \pi). \quad (2.4.4)$$

2.4.1.1 Symmetry at $\Gamma_1 = U$

The symmetry at U is described by its little group, whose generators can be chosen as I , G_z , and M_y . The representation matrices satisfy

$$U_U^{G_z} U_U^I = U_U^I U_U^{G_z}, \quad U_U^{G_z} U_U^{M_y} = -U_U^{M_y} U_U^{G_z}, \quad U_U^{M_y} U_U^I = U_U^I U_U^{M_y}. \quad (2.4.5)$$

In order to discuss topological invariants, we are interested in the information of simultaneous eigenstates of G_z and I . Therefore, let us start from the Abelian subgroup $\{E, G_z, I, G_z I\}$, whose irreducible representations are four one-dimensional representations (that is, simultaneous eigenstates of G_z and I), $\gamma_{\pm, g(u)}$ in Table 2.3. By adding M_y , the representations $\gamma_{\pm, g}$ are paired up to become E_g , while $\gamma_{\pm, u}$ to become E_u . This leads to the relations ⁴

$$N_{\pm, g}^{\text{occ.}}(U) = N_{\mp, g}^{\text{occ.}}(U), \quad N_{\pm, u}^{\text{occ.}}(U) = N_{\mp, u}^{\text{occ.}}(U). \quad (2.4.6)$$

Accordingly, we obtain

$$N_{+, u}^{\text{occ.}}(U) + N_{-, -\eta_I}^{\text{occ.}}(U) = \begin{cases} 2N_{+, u}^{\text{occ.}}(U) & (\eta_I = +1) \\ N^{\text{occ.}}(U)/2 & (\eta_I = -1) \end{cases}, \quad (2.4.7a)$$

$$N_{\pm}^{\text{occ.}}(U) = N_{\mp}^{\text{occ.}}(U) = N^{\text{occ.}}(U)/2. \quad (2.4.7b)$$

		G_z	I	M_y
E_g	$\gamma_{+, g}$	+1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{-, g}$	-1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
E_u	$\gamma_{+, u}$	+1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{-, u}$	-1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Table 2.3: Generators of the little group and irreducible representations at U point.

2.4.1.2 Symmetry at $\Gamma_2 = R$

At $\Gamma_2 = R$, the representation matrices satisfy

$$U_R^{G_z} U_R^I = U_R^I U_R^{G_z}, \quad U_R^{G_z} U_R^{M_y} = -U_R^{M_y} U_R^{G_z}, \quad U_R^{M_y} U_R^I = -U_R^I U_R^{M_y}. \quad (2.4.8)$$

In this case, irreducible representations of $\{E, G_z, I, G_z I\}$ are paired up to E_1 and E_2 in Table. 2.4. This leads to the identity

⁴Note that time-reversal symmetry trivially doubles the dimension of irreducible representations, since it keeps inversion and glide eigenvalues at Γ_i .

		G_z	I	M_y
E_1	$\gamma_{+,g}$	+1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{-,u}$	-1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
E_2	$\gamma_{+,u}$	+1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{-,g}$	-1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Table 2.4: Generators of the little group and irreducible representations at R point.

$$N_{\pm,g}^{\text{occ.}}(R) = N_{\mp,u}^{\text{occ.}}(R). \quad (2.4.9)$$

By using this, we obtain

$$N_{+,u}^{\text{occ.}}(R) + N_{-,-\eta_I}^{\text{occ.}}(R) = \begin{cases} N^{\text{occ.}}(R)/2 & (\eta_I = +1) \\ 2N_{+,u}^{\text{occ.}}(R) & (\eta_I = -1) \end{cases}, \quad (2.4.10a)$$

$$N_{\pm}^{\text{occ.}}(R) = N_{\mp}^{\text{occ.}}(R) = N^{\text{occ.}}(R)/2. \quad (2.4.10b)$$

2.4.1.3 Occupation number formulas for G_z

From the symmetry analysis, we obtain the following results for $\mathbb{Z}_4$ and $\mathbb{Z}_2$ invariants. For $\eta_I = +1$, $\mathbb{Z}_4$ invariant reduces to

$$\theta_4(\pi) = 2(2N_{+,u}^{\text{occ.}}(U) + N^{\text{occ.}}(R)/2) = N^{\text{occ.}}(R) \pmod{4}. \quad (2.4.11)$$

For $\eta_I = -1$, $\mathbb{Z}_4$ invariant reduces to

$$\theta_4(\pi) = 2(N^{\text{occ.}}(U)/2 + 2N_{+,u}^{\text{occ.}}(R)) = N^{\text{occ.}}(U) \pmod{4}. \quad (2.4.12)$$

The $\mathbb{Z}_2$ invariant for $\eta_I = -1$ is given by

$$\nu_{\pm}(\pi) = N^{\text{occ.}}(U)/2 + N^{\text{occ.}}(R)/2 \pmod{2} \quad (2.4.13a)$$

$$= N^{\text{occ.}}(U)/2 - N^{\text{occ.}}(R)/2 \pmod{2} \quad (2.4.13b)$$

$$= \#\text{FS}_{R \rightarrow U}/4 \pmod{2} \quad (2.4.13c)$$

Here, we defined

$$\#\text{FS}_{\Gamma_1 \rightarrow \Gamma_2} = \int_{\Gamma_1 \rightarrow \Gamma_2} d\mathbf{k} \cdot \nabla_{\mathbf{k}} M^{\text{occ.}}(\mathbf{k}). \quad (2.4.14)$$

with $M^{\text{occ.}}(\mathbf{k})$ the number of occupied states at $\mathbf{k}$ including Kramers degeneracy. In particular, $M^{\text{occ.}}(\Gamma_i) = 2N^{\text{occ.}}(\Gamma_i)$. Since $\nabla_{\mathbf{k}} M^{\text{occ.}}(\mathbf{k})$ is finite only at the Fermi surfaces, $\#\text{FS}_{\Gamma_1 \rightarrow \Gamma_2}$ is the number of Fermi surfaces counted with sign between two points Γ_1 and Γ_2 . For example, when going out of an hole (electron) Fermi surface around Γ_1 , there is a contribution $+2$ (-2) to the integral, including ΘI degeneracy.

2.4.2 Topological invariants by G_x

Next, we consider topological invariants ensured by $G_x = \{ M_x \mid (\hat{x} + \hat{y} + \hat{z})/2 \}$ symmetry. In this case, we set $\mathbf{a} = \hat{y} + \hat{z}$, $\mathbf{b} = \hat{z}$, and $\mathbf{c} = \hat{x}$, while $k_a = \mathbf{k} \cdot \mathbf{a} = k_y + k_z$, $k_b = k_z$, and $k_c = k_x$. Accordingly, we obtain

$$\Gamma_1 : S = (\pi, \pi, 0), \quad \Gamma_2 : U = (\pi, 0, \pi). \quad (2.4.15)$$

2.4.2.1 Symmetry at S

Let us choose the generators of the little group at S to G_x , I , and M_y . The representation matrices satisfy

$$U_S^{G_x} U_S^I = U_S^I U_S^{G_x}, \quad U_S^{G_x} U_S^{M_y} = U_S^{M_y} U_S^{G_x}, \quad U_S^{M_y} U_S^I = -U_S^I U_S^{M_y}. \quad (2.4.16)$$

Thus, the one-dimensional representations of the Abelian subgroup $\{ E, G_x, I, G_x I \}$ are paired up to E_+ and E_- as in Table 2.5. We obtain the following relations:

$$N_{\pm, g}^{\text{occ.}} = N_{\pm, u}^{\text{occ.}}, \quad (2.4.17)$$

and accordingly,

$$N_{+, u}^{\text{occ.}}(S) + N_{-, -\eta_I}^{\text{occ.}}(S) = \begin{cases} N^{\text{occ.}}(S)/2 & (\eta_I = +1) \\ N^{\text{occ.}}(S)/2 & (\eta_I = -1) \end{cases}, \quad (2.4.18a)$$

$$N_{\pm}^{\text{occ.}}(S) = 2N_{\pm, g}^{\text{occ.}}(S). \quad (2.4.18b)$$

		G_x	I	M_y
E_+	$\gamma_{+, g}$	+1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{+, u}$	+1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
E_-	$\gamma_{-, g}$	-1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{-, u}$	-1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Table 2.5: Generators of the little group and irreducible representations at S point.

2.4.2.2 Symmetry at U

Let us choose the generators of the little group at U as G_x , I , and M_y . The representation matrices satisfy

$$U_U^{G_x} U_U^I = U_U^I U_U^{G_x}, \quad U_U^{G_x} U_U^{M_y} = -U_U^{M_y} U_U^{G_x}, \quad U_U^{M_y} U_U^I = U_U^I U_U^{M_y}. \quad (2.4.19)$$

The representations of the Abelian subgroup $\{ E, G_x, I, G_x I \}$ are paired up as in Table. 2.6. Thus, we obtain

$$N_{\pm, g(u)}^{\text{occ.}} = N_{\mp, g(u)}^{\text{occ.}}, \quad (2.4.20)$$

and accordingly,

$$N_{+, u}^{\text{occ.}}(U) + N_{-, -\eta_I}^{\text{occ.}}(U) = \begin{cases} 2N_{+, u}^{\text{occ.}}(U) & (\eta_I = +1) \\ N^{\text{occ.}}(U)/2 & (\eta_I = -1) \end{cases}, \quad (2.4.21a)$$

$$N_{\pm}^{\text{occ.}}(U) = N^{\text{occ.}}(U)/2. \quad (2.4.21b)$$

		G_x	I	M_y
E_g	$\gamma_{+, g}$	+1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{-, g}$	-1	+1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
E_u	$\gamma_{+, u}$	+1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
	$\gamma_{-, u}$	-1	-1	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Table 2.6: Generators of the little group and irreducible representations at U point.

2.4.2.3 Occupation number formulas for G_x

From the symmetry analysis, we obtain the following results for $\mathbb{Z}_4$ and $\mathbb{Z}_2$ invariants. For $\eta_I = +1$, $\mathbb{Z}_4$ invariant reduces to

$$\theta_4(\pi) = 2(N^{\text{occ.}}(S)/2 + 2N_{+, u}^{\text{occ.}}(U)) = N^{\text{occ.}}(S) \pmod{4}. \quad (2.4.22)$$

For $\eta_I = -1$, $\mathbb{Z}_4$ invariant reduces to

$$\theta_4(\pi) = 2(N^{\text{occ.}}(S)/2 + N^{\text{occ.}}(U)/2) = \#\text{FS}_{S \rightarrow U}/2 \pmod{4}. \quad (2.4.23)$$

$\mathbb{Z}_2$ invariant for $\eta_I = -1$ is obtained by

$$\nu_{\pm}(\pi) = 2N_{\pm, g}^{\text{occ.}}(S) + N^{\text{occ.}}(U)/2 = N^{\text{occ.}}(U)/2 \pmod{2}. \quad (2.4.24)$$

2.5 Summary of the formulas for glide topological invariants in space group $Pnma$

Here, we summarize the formulas obtained in the previous sections. In time-reversal symmetric 3D superconductors with glide symmetry, topological invariants ensured by glide symmetry are defined on the two glide-invariant planes specified by $k_c = 0, \pi$ when glide symmetry

is written as $G = \{ G_c \mid \mathbf{a}/2 + \mathbf{c}/2 \}$. We can define $\mathbb{Z}_4$ invariants $\theta_4(k_c = 0)$ and $\theta_4(k_c = \pi)$ for glide-odd superconductivity, while $\mathbb{Z}_2$ invariants $\nu_\pm(k_c = 0)$ and $\nu_\pm(k_c = \pi)$ for glide-even superconductivity. In Sec. 2.3, we have shown that the glide topological invariants $\theta_4(\pi)$ and $\nu_\pm(\pi)$ can be simplified when we have a screw symmetry sharing the axis with the glide symmetry. On the other hand, we have not obtained such simplified formulas for the remaining topological invariants defined on the basal plane $k_c = 0$, and thus numerical calculations are required to evaluate them. In Sec. 2.4, the topological invariants defined on the zone face $k_c = \pi$ are shown to be further simplified by considering the full symmetry of the space group $Pnma$, to which UCoGe belongs. The results are summarized in Table 2.7. Here, $M^{\text{occ.}}(\Gamma_i)$ is

	Glide parity	Topological invariants
G_z	Odd (A_u, B_{1u})	$\theta_4^{(z)}(\pi) = M^{\text{occ.}}(U)/2 = \#\text{FS}_{R \rightarrow U}/2 + \Delta M(R)$
	Even (B_{2u}, B_{3u})	$\nu_\pm^{(z)}(\pi) = \#\text{FS}_{R \rightarrow U}/4$
G_x	Odd (A_u, B_{3u})	$\theta_4^{(x)}(\pi) = \#\text{FS}_{S \rightarrow U}/2$
	Even (B_{1u}, B_{2u})	$\nu_\pm^{(x)}(\pi) = M^{\text{occ.}}(U)/4 = \#\text{FS}_{R \rightarrow U}/4 + \Delta M(S)/2$

Table 2.7: Summary of the results of topological invariants. $\mathbb{Z}_4$ and $\mathbb{Z}_2$ invariants are evaluated with modulo four and two, respectively. Here, $\Delta M(\Gamma_i) = M^{\text{occ.}}(\Gamma_i)/2 = 2(N_{+u}^{\text{occ.}}(\Gamma_i) - N_{-u}^{\text{occ.}}(\Gamma_i))$ with $\Gamma_i = R, S$ represents the deviation from the SU(2) symmetric case shown in Table 2.8.

the number of occupied electron states at Γ_i including Kramers degeneracy. $\#\text{FS}_{\Gamma_1 \rightarrow \Gamma_2}$ is the number of Fermi surfaces (including Kramers degeneracy) counted with sign; for example, when going out of an hole (electron) Fermi surface around Γ_1 , there is a contribution $+2$ (-2) to the integral, including ΘI degeneracy.

The results shown in Table 2.7 are rigorous for general situations and topological invariants are easily estimated with the help of first-principles calculations. However, it is also desirable to relate $M^{\text{occ.}}(U)$ to the number of Fermi surfaces, since we can visually (and easily) determine topological invariants. For this reason, let us translate $\theta_4^{(z)}(\pi)$ and $\nu_\pm^{(x)}(\pi)$ into the language of Fermi surfaces. As shown in the rightmost column, $\theta_4^{(z)}(\pi)$ and $\nu_\pm^{(x)}(\pi)$ are given not only by $\#\text{FS}$ but also by correction term ΔM . We can show that ΔM physically corresponds to the correction by strong spin-orbit coupling and vanish in the SU(2) limit.

Let us consider the case of small effective spin-orbit coupling of the energy bands near Fermi energy. In this case, we have SU(2) symmetry of the Kramers degree of freedom of the bands. Glide eigenvalues can be switched by SU(2) rotation, and we can show that R and S

points are eight-fold degenerate: $M^{\text{occ.}}(R), M^{\text{occ.}}(S) \in 8\mathbb{Z}$.⁵ Thus, we obtain

$$M^{\text{occ.}}(U) = M^{\text{occ.}}(U) - M^{\text{occ.}}(R) + M^{\text{occ.}}(R) = \#\text{FS}_{R \rightarrow U} \pmod{8}, \quad (2.5.2a)$$

$$M^{\text{occ.}}(U) = M^{\text{occ.}}(U) - M^{\text{occ.}}(S) + M^{\text{occ.}}(S) = \#\text{FS}_{S \rightarrow U} \pmod{8}. \quad (2.5.2b)$$

Accordingly, we obtain Table 2.8 for SU(2) symmetric cases. Practically speaking, weak

	Glide parity	Topological invariants
G_z	Odd (A_u, B_{1u})	$\theta_4^{(z)}(\pi) = \#\text{FS}_{R \rightarrow U}/2$
	Even (B_{2u}, B_{3u})	$\nu_{\pm}^{(z)}(\pi) = \#\text{FS}_{R \rightarrow U}/4$
G_x	Odd (A_u, B_{3u})	$\theta_4^{(x)}(\pi) = \#\text{FS}_{S \rightarrow U}/2$
	Even (B_{1u}, B_{2u})	$\nu_{\pm}^{(x)}(\pi) = \#\text{FS}_{S \rightarrow U}/4$

Table 2.8: Summary of the results of topological invariants for SU(2) symmetric cases. $\mathbb{Z}_4$ and $\mathbb{Z}_2$ invariants are evaluated with modulo four and two, respectively.

or moderate effective spin-orbit coupling could be judged from the splitting of the Fermi surfaces at $k_c = \pi$ for $G = \{M_c \mid \mathbf{a}/2 + \mathbf{c}/2\}$. Indeed, if the system has SU(2) symmetry, we obtain an entire four-fold degeneracy of the bands at $k_c = \pi$, due to the screw symmetry $S = \{C_{2c} \mid \mathbf{a}/2 + \mathbf{c}/2\}$ accompanied by G with $S = IG$ ⁶. Therefore, if the splitting of the Fermi surfaces is small, we may use Table 2.8. Although Table 2.8 gives a convenient way to estimate topological invariants, it should be noted that Table 2.7 should be used to make a final conclusion.

For completeness, we also summarize in Table 2.9 topological invariants of even-parity superconductivity, although the results are not relevant to UCoGe. $\mathbb{Z}_4$ invariants may also be nontrivial for even-parity superconductivity, while $\mathbb{Z}_2$ invariants are always trivial. These results point to an interesting possibility of $\mathbb{Z}_4$ topological superconductivity in nonsymmorphic d -wave superconductors, which we leave as a future issue.

2.6 Application to UCoGe

In this section, we demonstrate that UCoGe is a promising candidate of $\mathbb{Z}_4$ and $\mathbb{Z}_2$ topological glide superconductivity, by using the Fermi-surface formulas and model calculations.

⁵Actually, we obtain for S and R points,

$$M^{\text{occ.}} = 2N^{\text{occ.}} = 4N_{+,g}^{\text{occ.}} = 8N_{+,g}^{\text{occ.}} \in 8\mathbb{Z}. \quad (2.5.1)$$

⁶Actually, each glide eigensector has degeneracy by ΘI , and glide eigenvalues can be flipped by SU(2) rotation [110].

	Glide parity	Topological invariants
G_z	Odd (B_{2g}, B_{3g})	$\theta_4^{(z)}(\pi) = M^{\text{occ.}}(R)/2$
	Even (A_g, B_{1g})	$\nu_{\pm}^{(z)}(\pi) = 0$
G_x	Odd (B_{1g}, B_{2g})	$\theta_4^{(x)}(\pi) = M^{\text{occ.}}(S)/2$
	Even (A_g, B_{3g})	$\nu_{\pm}^{(x)}(\pi) = 0$

Table 2.9: Summary of the results of topological invariants obtained for even-parity superconductivity. $\mathbb{Z}_4$ and $\mathbb{Z}_2$ invariants are evaluated with modulo four and two, respectively.

2.6.1 Application of the Fermi-surface formulas to UCoGe

Let us apply the Fermi-surface formulas to UCoGe. The pairing symmetry of UCoGe has not been experimentally identified yet, and therefore, we consider all the pairing symmetry for completeness. Fermi surfaces of UCoGe have been obtained from first-principles calculations done by two groups [9, 10, 11]. Here, we take one of the results [9, 10] as an example to demonstrate topological glide superconductivity in UCoGe. Topological invariants for the other study [11] are discussed later.

Fermi surfaces of UCoGe given in Fig. 26 (i) of Ref. [10] consist of two cylinder-shaped electron Fermi surfaces around the $S - R$ line, electron pockets around X point, and hole pockets around Y point. There is also a tiny electron pocket around Γ point. In the following, we refer to these Fermi surfaces as "Fermi surfaces of Ref. [9, 10]". Let us consider topological invariant $\theta_4^{(x)}(\pi)$ defined for A_u and B_{3u} pairing symmetries shown in Table 2.10. According to Table 2.7, $\theta_4^{(x)}(\pi)$ is determined by the number of Fermi surfaces between S and U points. There are two electron Fermi surfaces on the straight line connecting S and U points, each of which is doubly degenerate by ΘI symmetry. Thus, we obtain $\#FS_{S \rightarrow U} = -4$, to conclude $\theta_4^{(x)}(\pi) = 2$. Note that arbitrary path can be chosen to evaluate topological invariants, as is clear from the definition of $\#FS_{\Gamma_1 \rightarrow \Gamma_2}$, Eq. (2.4.13c).

The other topological invariants can be obtained in the same way, by using Table 2.8. We summarize the results in Table 2.11. Surprisingly, all the $\mathbb{Z}_4$ and $\mathbb{Z}_2$ topological invariants

IR	Symmetries				d vector
	I	G_z	M_y	G_x	
A_u	-1	-1	-1	-1	$k_x \hat{x}, k_y \hat{y}, k_z \hat{z}$
B_{1u}	-1	-1	+1	+1	$k_y \hat{x}, k_x \hat{y}$
B_{2u}	-1	+1	-1	+1	$k_z \hat{x}, k_x \hat{z}$
B_{3u}	-1	+1	+1	-1	$k_z \hat{y}, k_y \hat{z}$

Table 2.10: Odd-parity irreducible representations of the point group D_{2h} . Characters are shown only for generators of D_{2h} . We also show typical d vectors.

IR	Topological invariants	
	G_z	G_x
A_u	$\theta_4^{(z)}(\pi) = 2$	$\theta_4^{(x)}(\pi) = 2$
B_{1u}	$\theta_4^{(z)}(\pi) = 2$	$\nu_{\pm}^{(x)}(\pi) = 1$
B_{2u}	$\nu_{\pm}^{(z)}(\pi) = 1$	$\nu_{\pm}^{(x)}(\pi) = 1$
B_{3u}	$\nu_{\pm}^{(z)}(\pi) = 1$	$\theta_4^{(x)}(\pi) = 2$

Table 2.11: Glide topological invariants evaluated for the Fermi surfaces of Ref. [9, 10].

are nontrivial for the Fermi surfaces of Ref. [9, 10] (Table 2.11 is reproduced by using the formulas in Table 2.7, because, $M^{\text{occ}}(U) = 70 \cdot 2 \in 8\mathbb{Z} + 4$ from Ref. [9]). In particular, three out of four irreducible representations have nontrivial $\mathbb{Z}_4$ indices. Thus, UCoGe is strongly suggested to be a $\mathbb{Z}_4$ topological superconductor, whose candidate materials have not been known.

The other topological invariants of 3D time-reversal symmetric superconductivity with glide symmetry can also be obtained from numerical calculations [111]. We have made a numerical calculation based on the model of cylinder Fermi surfaces presented in Sec. 2.6.2, and obtained Table 2.12. In Table 2.12, the analytical results in Table 2.11 are correctly reproduced. In particular, UCoGe has nontrivial strong glide indices related to G_x , while weak indices for G_z . This is naturally understood as a result of three-dimensional (two-dimensional) nature of the cylinder Fermi surfaces in $\hat{x}$ ($\hat{z}$) direction.

IR	Topological invariants	
	G_z	G_x
A_u	(0, 0, 2)	(0, 1, 0)
B_{1u}	(0, 0, 2)	{ 0, 1, 0 }
B_{2u}	{ 0, 0, 1 }	{ 0, 1, 0 }
B_{3u}	{ 0, 0, 1 }	(0, 1, 0)

Table 2.12: Numerical results of topological invariants of UCoGe. Calculation is based on the model in Sec. 2.6.2. Here, round braces represent glide-odd index $(\mathbb{Z}^W, \mathbb{Z}_2^{\text{strong}}, \mathbb{Z}_4^{\text{weak}})$, while square braces represent glide-even index $\{\mathbb{Z}_2^{\text{CS}_T}, \mathbb{Z}_2^{\text{strong}}, \mathbb{Z}_2^{\text{weak}}\}$. For notations, see Sec. 2.2.4.

Although we have obtained $W = 0$ for the model in Sec. 2.6.2, the even-integer part of W is model dependent in general. Winding number contributed by the cylinder Fermi surfaces should be equal to either $W \in 4\mathbb{Z}$ or $W \in 4\mathbb{Z} + 2$, by considering the number of Fermi surfaces [57, 108]. Thus, topological classification of the A_u states is obtained as Table 2.13. Note that classification of the other pairing symmetries does not have ambiguity of winding number, since it vanishes in the presence of even-glide or even-mirror symmetry (a proof is

available in Ref. [111]).

IR	Topological invariants	
	G_z	G_x
A_u	$(4n, 0, 2)$ $(4n + 2, 1, 0)$	$(4n, 1, 0)$ $(4n + 2, 0, 2)$
B_{1u}	$(0, 0, 2)$	$\{0, 1, 0\}$
B_{2u}	$\{0, 0, 1\}$	$\{0, 1, 0\}$
B_{3u}	$\{0, 0, 1\}$	$(0, 1, 0)$

Table 2.13: Topological invariants of UCoGe contributed by cylinder Fermi surfaces with n an arbitrary integer depending on the details of Fermi surfaces and gap function. Here, round braces represent glide-odd index $(\mathbb{Z}^W, \mathbb{Z}_2^{\text{strong}}, \mathbb{Z}_4^{\text{weak}})$, while square braces represent glide-even index $\{\mathbb{Z}_2^{\text{CS}_T}, \mathbb{Z}_2^{\text{strong}}, \mathbb{Z}_2^{\text{weak}}\}$. For notations, see Sec. 2.2.4.

Let us discuss topological invariants carried by the other Fermi surfaces. First, we consider the A_u representation. The tiny Γ Fermi surfaces would carry odd-integer winding number since there is one pair of Kramers degenerate Fermi surfaces [57, 108]. The value of the winding number is expected to be $W = \pm 1$, in analogy with the B-phase of ^3He . The Γ Fermi surface is also expected to carry $\theta_4^{(z)}(0) = \pm 1$ or ∓ 1 , since one pair of Kramers degenerate Fermi surfaces cross the $\Gamma - Y$ line, where $\mathbb{Z}_2$ part of $\theta_4^{(z)}(0)$ is defined [5]. The same thing can be said about $\theta_4^{(x)}(0)$. Thus, when $(W, \theta_4(0)) = (\pm 1, \pm 1)$ is added, $\mathbb{Z}^W$ changes by ± 1 and other indices remain unchanged. On the other hand, addition of $(W, \theta_4(0)) = (\pm 1, \mp 1)$ changes $(\mathbb{Z}^W, \mathbb{Z}_2^{\text{strong}}, \mathbb{Z}_4^{\text{weak}})$ by $(\pm 1, 1, 2)$. The other Fermi surfaces around X and Y points are expected to be irrelevant to topological invariants, since they do not enclose time-reversal invariant momenta. Thus, the A_u state of UCoGe is classified into topological superconductivity with winding number and either strong or weak glide indices.

The other pairing symmetries, B_{1u} , B_{2u} , and B_{3u} should have point nodes on the Γ Fermi surfaces. This is because, on one hand, W should be an odd integer, but on the other hand, W should vanish due to even mirror or glide symmetry. This inconsistency is resolved only when there are excitation nodes. Indeed, point nodes on the Γ Fermi surfaces are also expected from a simple symmetry analysis [15]. Even in the presence of point nodes, glide topological invariants defined on the Brillouin zone faces remain valid and corresponding topological surface states appear. We discuss this point in Sec. 2.7.2.

2.6.2 Minimal model for UCoGe

In order to establish the validity of our Fermi-surface formulas, we made a minimal model of UCoGe, which mimics the cylinder-like Fermi surfaces obtained by Ref. [9, 10]. We consider a single-orbital tight-binding model on the Uranium sites of UCoGe. There are four Uranium

atoms in a unit cell, as shown in Fig. 2.1. We label the atoms as $a1, a2, b1$, and $b2$, and introduce Pauli matrices η_μ and σ_μ , with $\eta_z = \pm 1$ and $\sigma_z = \pm 1$ specifying the label a, b and $1, 2$, respectively. Electron spins are described by the Pauli matrix s_μ . Normal state Hamiltonian is given by

$$H_{N,\mathbf{k}} = H_{\text{hop},\mathbf{k}} + H_{\text{SOC},\mathbf{k}}, \quad (2.6.1)$$

where the hopping part $H_{\text{hop},\mathbf{k}}$ is given by

$$H_{\text{hop},\mathbf{k}} = s_0 \otimes \begin{pmatrix} H_{a,\mathbf{k}} & H_{ab,\mathbf{k}} \\ H_{ab,\mathbf{k}}^\dagger & H_{b,\mathbf{k}} \end{pmatrix}_\eta, \quad (2.6.2a)$$

$$H_{a,\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k}} & \epsilon_{12,\mathbf{k}} \\ \epsilon_{12,\mathbf{k}}^* & \epsilon_{\mathbf{k}} \end{pmatrix}_\sigma, \quad H_{b,\mathbf{k}} = H_{a,\mathbf{k}}^T, \quad H_{ab,\mathbf{k}} = \text{diag}(v_{1,\mathbf{k}}, v_{2,\mathbf{k}})_\sigma, \quad (2.6.2b)$$

and spin-orbit-coupling part $H_{\text{SOC},\mathbf{k}}$ is given by

$$H_{\text{SOC},\mathbf{k}} = \mathbf{g}_{\mathbf{k}} \cdot \mathbf{s} \sigma_z \eta_z + \mathbf{g}'_{\mathbf{k}} \cdot \mathbf{s} \eta_z. \quad (2.6.3)$$

The scalar functions appearing above are given by

$$\epsilon_{\mathbf{k}} = 2t'_1 \cos k_x + 2t_2 \cos k_y + 2t_3 \cos k_z - \mu, \quad \epsilon_{12,\mathbf{k}} = t_1(1 + e^{-ik_x}), \quad (2.6.4a)$$

$$v_{1,\mathbf{k}} = e^{-ik_x}(1 + e^{-ik_y})(t_{ab} + e^{ik_z}t'_{ab}), \quad v_{2,\mathbf{k}} = e^{ik_z}(1 + e^{-ik_y})(t_{ab} + e^{-ik_z}t'_{ab}), \quad (2.6.4b)$$

$$\mathbf{g}_{\mathbf{k}} = \alpha(-\sin k_y, \delta_\alpha \sin k_x, 0)^T, \quad \mathbf{g}'_{\mathbf{k}} = \beta(0, \delta_\beta \sin k_z, \sin k_y)^T, \quad (2.6.4c)$$

with parameters

$$(t_1, t_2, t_3, t_{ab}, t'_{ab}, \mu, t'_1, \alpha, \delta_\alpha, \beta, \delta_\beta) = (1, 0.2, 0.1, 0.5, 0.1, 0.55, 0.1, 0.3, 0.5, 0.3, 0.5) \quad (2.6.5)$$

to give cylinder-like Fermi surface shown in Fig. 2.2. In the following calculations of surface states, the size of the slab is set to $L_a = 200$ for $\mathbf{a}$ direction with periodic boundary condition while $L_b = 50$ for $\mathbf{b}$ direction with open boundary condition.

We adopt order parameters for each pairing symmetry as in Table 2.14. Here, we choose the direction of the $\mathbf{d}$ vector perpendicular to the $\hat{z}$ axis, which is the easy-magnetization axis of UCoGe. Most of the order parameters are chosen to be intra-sublattice, i.e. diagonal in both η and σ space, for simplicity. The δ term in B_{2u} is one of the simplest inter-sublattice (intra-chain) terms, i.e. offdiagonal in σ space, which is introduced to remove accidental nodes from glide invariant planes. We set $\delta = 1$ and also set the magnitude of the order parameter $d_0 = 0.5$, for visibility of surface state spectrum. It can be easily checked that these order parameters are compatible with the symmetries of $Pnma$, whose representation

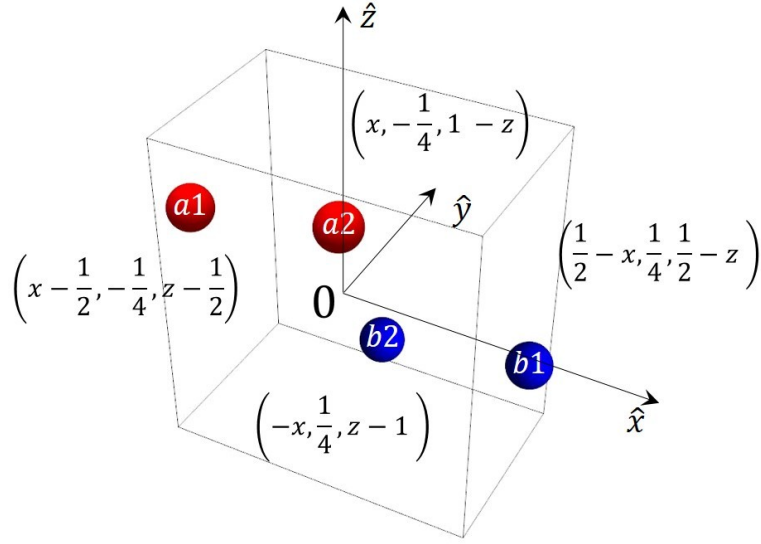


Figure 2.1: Uranium atom configuration of UCoGe with $(x, z) = (0.0101, 0.7075)$ [105]. Lattice constants are normalized to unity.

IR	$\Delta_{\mathbf{k}}/d_0$
A_u	$\sin k_x s_x + \sin k_y s_y + \sin k_z s_z \sigma_z$
B_{1u}	$\sin k_x s_y + \sin k_y s_x + \sin k_z s_y \sigma_z$
B_{2u}	$\sin k_x s_x \sigma_z + \sin k_y s_y \sigma_z + \sin k_z s_x + \delta \{ (1 + \cos k_x) s_x \sigma_y \eta_z - \sin k_x s_x \sigma_x \} / 2$
B_{3u}	$\sin k_x s_y \sigma_z + \sin k_y s_x \sigma_z + \sin k_z s_y$

Table 2.14: Model order parameters.

matrices are generated by

$$U_{\mathbf{k}}^I = \eta_x, \quad U_{\mathbf{k}}^{G_z} = -i s_z \otimes \begin{pmatrix} \begin{pmatrix} 0 & e^{-ik_x} \\ 1 & 0 \end{pmatrix}_{\sigma} & 0 \\ 0 & \begin{pmatrix} 0 & e^{ik_z} \\ e^{-ik_x + ik_z} & 0 \end{pmatrix}_{\sigma} \end{pmatrix}_{\eta}, \quad (2.6.6a)$$

$$U_{\mathbf{k}}^{G_x} = -i s_x \otimes \begin{pmatrix} 0 & \begin{pmatrix} 0 & e^{ik_x - ik_y} \\ e^{-ik_y} & 0 \end{pmatrix}_{\sigma} \\ \begin{pmatrix} 0 & e^{-ik_z} \\ e^{ik_x - ik_z} & 0 \end{pmatrix}_{\sigma} & 0 \end{pmatrix}_{\eta}. \quad (2.6.6b)$$

The model has point nodes (off glide invariant planes) for B_{2u} and B_{3u} states, while it is gapful for A_u and B_{1u} state. These nodes are accidental, in the sense that their presence is not ensured by symmetry. Their existence depends on the detailed $\mathbf{k}$ dependence of the order parameter as well as normal state Hamiltonian, and would be the artifact of our model:

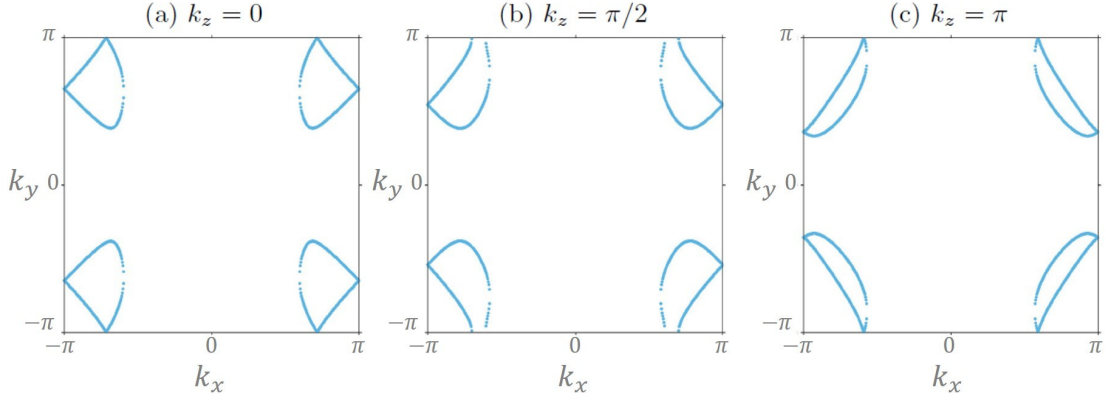


Figure 2.2: Slices of model Fermi surfaces at $k_z = 0, \pi/2$, and π .

Actually, some of them can be pair annihilated by tuning the order parameter, while the others are protected by accidental symmetry of our (over-simplified) model. For this reason, we do not discuss these nodes in the following.

2.6.3 Model calculation of surface states of topological G_z superconductivity

Let us discuss surface states of topological glide superconductivity protected by

$$G_z = \{ M_z \mid \hat{x}/2 + \hat{z}/2 \}. \quad (2.6.7)$$

In this case, $\mathbf{a} \times \mathbf{c} = \hat{y}$, and therefore, topological surface states appear at (010) and (0 $\bar{1}$ 0) surfaces.

2.6.3.1 Surface states of G_z -odd superconductivity

We consider G_z -odd superconductivity A_u and B_{1u} . In Fig. 2.3 (a) and (b), we show the (010) surface states at $k_z = \pi$ for A_u and B_{1u} states, respectively. Surface states with positive and negative glide eigenvalues are highlighted with red and blue, respectively. We have two helical modes, and thus obtain the result consistent with the prediction $\theta_4^{(z)}(\pi) = 2$.

It should be noted that the degeneracy of the surface states with positive and negative glide eigenvalues at $k_x = \pi$ is the artifact of our model. Actually, the degeneracy is lifted by a perturbation preserving the relevant symmetries (i.e. time-reversal, particle-hole, and G_z symmetries), as shown in Fig. 2.3 (c) and (d). Here, we added to $H_{\text{BdG},\mathbf{k}}|_{k_c=\pi}$ the following term:

$$\Delta H_{\text{BdG},\mathbf{k}} = \epsilon(U_{\mathbf{k}}^{G_z} + [U_{\mathbf{k}}^{G_z}]^\dagger)\tau_z \quad (\epsilon = 0.015) \quad (2.6.8)$$

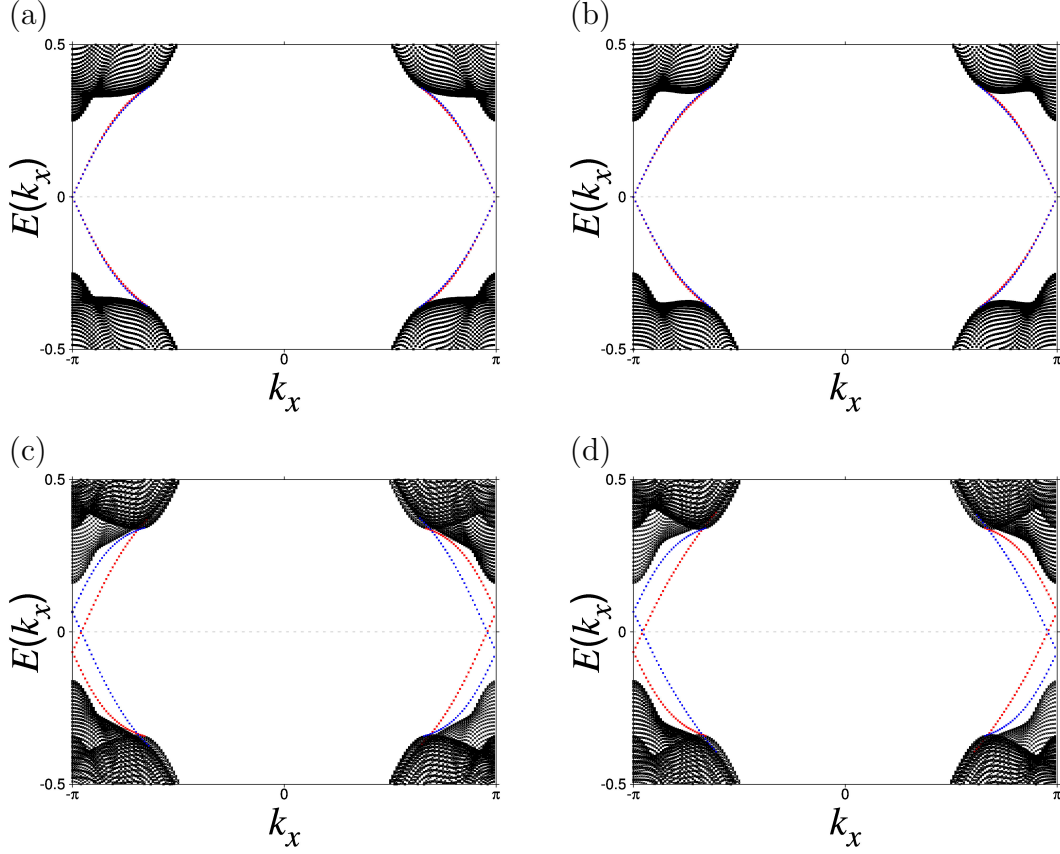


Figure 2.3: Topological surface states of G_z -odd superconductivity calculated for the model corresponding to $H_{\text{BdG},\mathbf{k}}$ (panel (a),(b)) and $H_{\text{BdG},\mathbf{k}} + \Delta H_{\text{BdG},\mathbf{k}}$ with $\Delta H_{\text{BdG},\mathbf{k}}$ given in Eq. (2.6.8) (panel (c),(d)). The panels (a) and (c) show the surface states of the A_u state, while the panels (b) and (d) show the surface states of the B_{1u} state.

This is consistent with the fact that gapless surface states ensured by the $\mathbb{Z}_4$ glide topological invariant are not necessarily pinned to $k_x = \pi$ [5], in contrast to those by the $\mathbb{Z}_2$ glide topological invariants illustrated in the next subsubsection.

2.6.3.2 Surface states of G_z -even superconductivity

We consider G_z -even superconductivity B_{2u} and B_{3u} . In Fig. 2.4 (a) and (b), we show the surface states for $k_z = \pi$. Red and blue states correspond to (010) surface states with positive and negative glide eigenvalues, respectively. In particular, it should be noticed that each eigensector has Kramers degenerate zero-energy states at $k_x = \pi$. This is consistent with the fact that glide eigensectors for glide-even superconductivity can be regarded as 1D class DIII topological superconductivity. Since these zero-energy states are protected by time-reversal, particle-hole, and even-glide symmetries, they should be stable against any

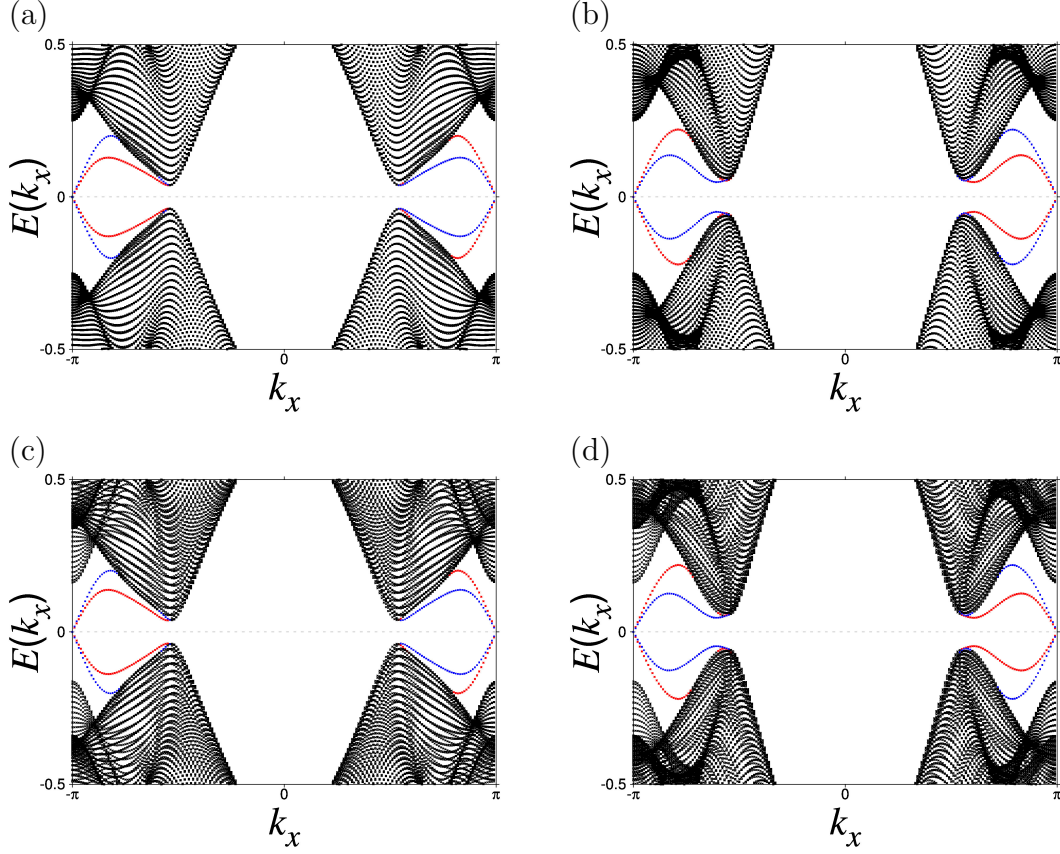


Figure 2.4: Topological surface states of G_z -even superconductivity calculated for the model corresponding to $H_{\text{BdG},\mathbf{k}}$ (panel (a),(b)) and $H_{\text{BdG},\mathbf{k}} + \Delta H_{\text{BdG},\mathbf{k}}$ with $\Delta H_{\text{BdG},\mathbf{k}}$ given in Eq. (2.6.8) (panel (c),(d)). The panels (a) and (c) show the surface states of the B_{2u} state, while the panels (b) and (d) show the surface states of the B_{3u} state.

perturbation preserving these relevant symmetries. Actually, they exist even when $\Delta H_{\text{BdG},\mathbf{k}}$ in Eq. (2.6.8) is added (panels (c) and (d) in Fig. 2.4), in stark contrast with glide-odd $\mathbb{Z}_4$ surface states in Fig. 2.3.

2.6.4 Model calculation of surface states of topological G_x superconductivity

Let us discuss surface states of topological glide superconductivity protected by

$$G_x = \{ M_x \mid (\hat{x} + \hat{y} + \hat{z})/2 \}. \quad (2.6.9)$$

In this case, $\mathbf{a} \times \mathbf{c} = -\hat{z} + \hat{y}$, and therefore, topological surface states appear at $(0\bar{1}1)$ and $(01\bar{1})$ surfaces.

2.6.4.1 Surface states of G_x -odd superconductivity

We consider G_x -odd superconductivity A_u and B_{3u} . In Fig. 2.5 (a) and (b), we show the $(0\bar{1}1)$ surface states for $k_c(=k_x) = \pi$. Surface states with positive and negative glide eigenvalues

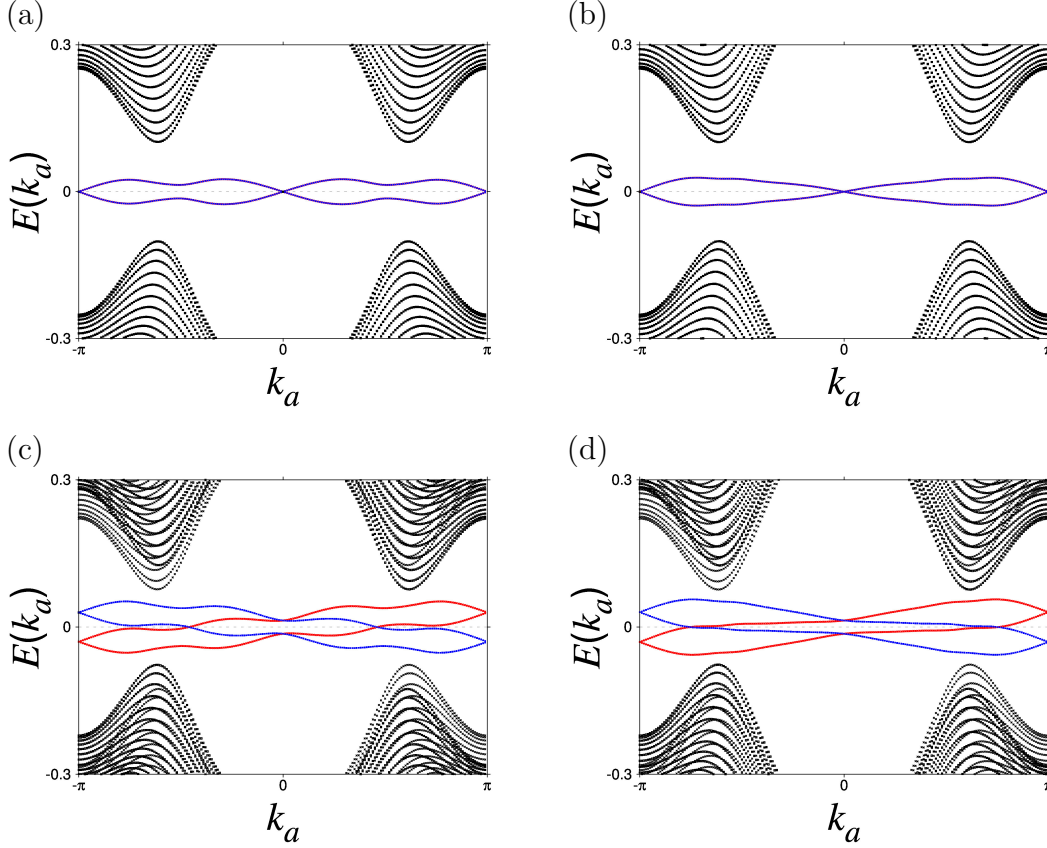


Figure 2.5: Topological surface states of G_x -odd superconductivity calculated for the model corresponding to $H_{\text{BdG},\mathbf{k}}$ (panel (a),(b)) and $H_{\text{BdG},\mathbf{k}} + \Delta H_{\text{BdG},\mathbf{k}}$ with $\Delta H_{\text{BdG},\mathbf{k}}$ given in Eq. (2.6.10) (panel (c),(d)). The panels (a) and (c) show the surface states of the A_u state, while the panels (b) and (d) show the surface states of the B_{3u} state.

are highlighted with red and blue, respectively. We have two helical modes, and thus obtain a result consistent with the prediction $\theta_4^{(x)}(\pi) = 2$.

As in the case of G_z topological superconductivity, the degeneracy at $k_a = \pi$ is the artifact of the model. We added the following term to $H_{\text{BdG},\mathbf{k}}|_{k_c=\pi}$ to obtain Fig. 2.5 (c) and (d):

$$\Delta H_{\text{BdG},\mathbf{k}} = \epsilon_1 (U_{\mathbf{k}}^{G_x} + [U_{\mathbf{k}}^{G_x}]^\dagger) \tau_z + \epsilon_2 s_x \sigma_y \eta_z \tau_x, \quad (\epsilon_1 = \epsilon_2 = 0.015). \quad (2.6.10)$$

Thus, the obtained surface states are consistent with $\theta_4^{(x)}(\pi) = 2$.

2.6.4.2 Surface states of G_x -even superconductivity

We consider G_x -even superconductivity B_{1u} and B_{2u} . In Fig. 2.6 (a) and (b), we show the $(0\bar{1}1)$ surface states for $k_c(=k_x) = \pi$. Surface states with positive and negative glide

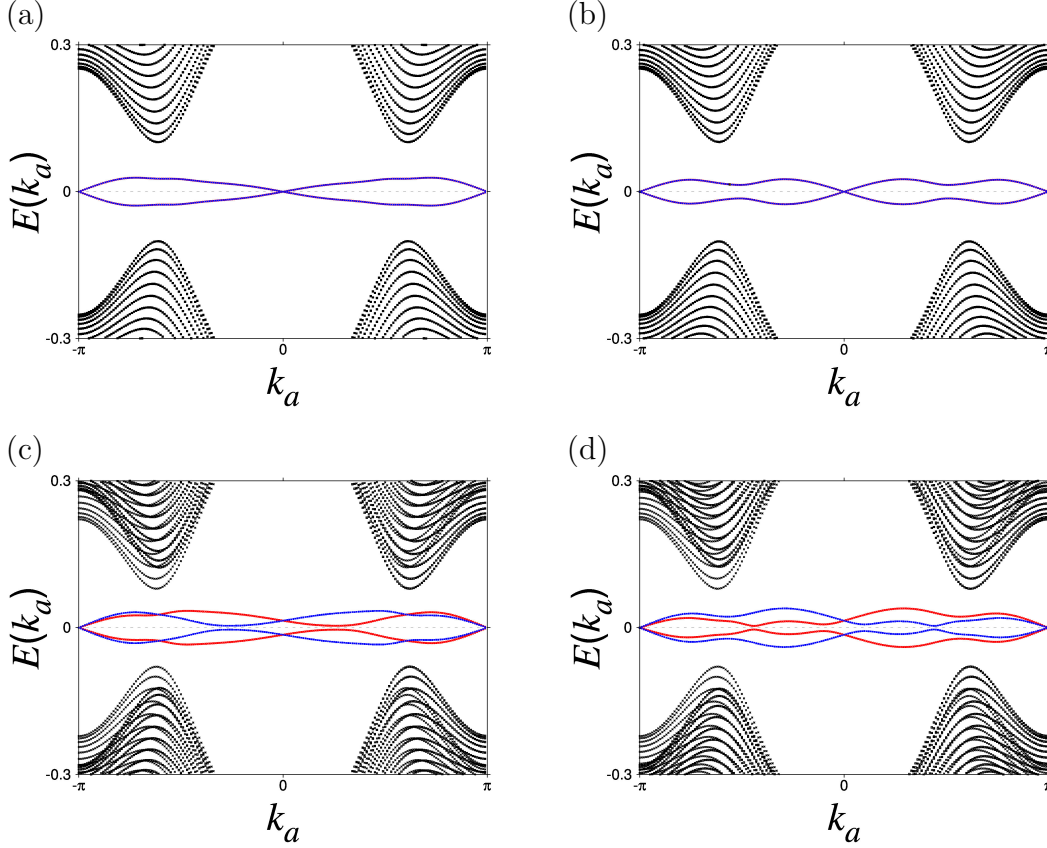


Figure 2.6: Topological surface states of G_x -even superconductivity calculated for the model corresponding to $H_{\text{BdG},\mathbf{k}}$ (panel (a),(b)) and $H_{\text{BdG},\mathbf{k}} + \Delta H_{\text{BdG},\mathbf{k}}$ with $\Delta H_{\text{BdG},\mathbf{k}}$ given in Eq. (2.6.10) (panel (c),(d)). The panels (a) and (c) show the surface states of the B_{1u} state, while the panels (b) and (d) show the surface states of the B_{2u} state.

eigenvalues are highlighted with red and blue, respectively. We have two helical modes, along with the zero-energy states at $k_a = \pi$ for both glide eigensectors. They are robust against the symmetry-preserving perturbation Eq. (2.6.10), as shown in Fig. 2.6 (c) and (d). Thus, we obtain the result consistent with the prediction $\nu_{\pm}^{(x)}(\pi) = 1$.

2.7 Discussion

In the previous sections, we have elucidated that UCoGe has nontrivial $\mathbb{Z}_4$ and $\mathbb{Z}_2$ indices for glide-odd and -even pairing symmetries, respectively, based on the formulas in Table 2.7

and Fermi surfaces obtained by first-principles calculations [9, 10]. In order to conclude the topology of the paramagnetic superconductivity in UCoGe under pressure, we have to discuss the following points:

1. Pairing symmetry of superconductivity in UCoGe under pressure.
2. Possibility and influence of excitation nodes.
3. Possibility and influence of deviation of Fermi surfaces from those by Ref. [9, 10].

Below, we discuss these points order by order.

2.7.1 Pairing symmetry of UCoGe under pressure

Among the odd-parity pairing symmetries, $\mathbb{Z}_4$ topological superconductivity is realized for A_u , B_{1u} , and B_{3u} states, while $\mathbb{Z}_2$ topological superconductivity is realized for B_{1u} , B_{2u} , and B_{3u} states. In order to determine the topology of UCoGe, and in particular, to identify the novel $\mathbb{Z}_4$ topological superconductivity, we have to discuss which pairing symmetry is likely to be realized in the paramagnetic superconducting phase of UCoGe.

Interestingly, the pairing symmetry of UCoGe may not be B_{2u} . Indeed, there is an experiment supporting the A_u representation of C_{2h} for the pairing symmetry in the ferromagnetic superconducting phase at ambient pressure: Temperature dependence of upper critical field agrees well with the theoretical calculation, demonstrating the importance of longitudinal ferromagnetic fluctuations [112]. Since superconducting transition temperature in the pressure-temperature phase diagram does not abruptly change across the ferromagnetic critical point [96, 100], it is natural to expect that the A_u state of C_{2h} in the ferromagnetic state smoothly connects into the corresponding irreducible representations of D_{2h} in the paramagnetic state, that is, A_u and B_{1u} states. Note that A_u and B_{1u} states are consistent with a naive expectation of the d vector in the ab plane (see Table 2.10), which is perpendicular to the c axis (the easy magnetization axis). d vector pinned to the ab plane is also suggested from a recent experiment by nuclear magnetic resonance (NMR) under pressure, showing only a small change of the Knight shift [104].

Thus, judging from the current situation, it is plausible to expect A_u or B_{1u} states, which are $\mathbb{Z}_4$ topological superconductivity according to our Fermi-surface formulas. Therefore, UCoGe is the first and most promising candidate of $\mathbb{Z}_4$ topological superconductivity, although further experimental effort is necessary to fully identify the pairing symmetry.

2.7.2 Possibility and influence of excitation nodes

In the above sections, we have basically assumed gapful energy spectrum, although possibility of the point nodes on the tiny Γ Fermi surfaces have already been discussed in

Sec. 2.6. Experimentally, line-nodal behavior has been reported in the ferromagnetic state by NMR/NQR [97, 113]. Possibility of line nodes has also been discussed by thermal transport measurements [114]. From a theoretical point of view, the line nodes of odd-parity superconductors, which are prohibited within point-group-symmetry analysis [15, 115], can be understood as those protected by nonsymmorphic space-group symmetry [110, 116, 117, 118, 119]. These line nodes in the ferromagnetic state are naturally expected to exist also in the paramagnetic superconducting phase [118]. Nodal excitations in the paramagnetic superconducting phase has been suggested by NMR, but further study is necessary [101]. Considering these experimental and theoretical backgrounds, nodal excitations in the paramagnetic superconductivity should be discussed as a realistic possibility.

In this subsection, we discuss what kind of nodes may exist and how topological properties and surface states are affected. To be specific, we discuss effect on glide topological invariants defined on $k_z = \pi$ and $k_x = \pi$ based on the Fermi surfaces given in Ref. [9, 10].

First, point nodes are expected to appear on the Γ Fermi surfaces and Y Fermi surfaces. However, their positions are off the $k_z = \pi$ and $k_x = \pi$ planes, and therefore are not harmful for $\theta_4^{(z)}(\pi)$ and $\nu_{\pm}^{(z)}(\pi)$ as well as $\theta_4^{(x)}(\pi)$ and $\nu_{\pm}^{(x)}(\pi)$. The X Fermi surfaces can also have point nodes, which is on the $k_x = \pi$ plane. However, they are off the $S-U$ line, and therefore $\nu_{\pm}^{(x)}(\pi)$ is unaffected. $\theta_4^{(x)}(\pi)$ and corresponding topological surface states may be affected by the point nodes, but zero-energy states may remain to exist, by taking a suitable surface direction.⁷

Next, we discuss effect of line nodes. It has been shown that line nodes are allowed to exist at the Brillouin zone face of mirror- or glide-odd superconductivity with screw symmetry. This is just the situation we are considering for simplified $\mathbb{Z}_4$ topological invariants. Accordingly, line nodes are predicted at the positions in Table 2.15 for each pairing symmetry. In

IR	Position of line nodes
A_u	$k_x = \pi, k_y = \pi, k_z = \pi$
B_{1u}	$k_z = \pi$
B_{2u}	$k_y = \pi$
B_{3u}	$k_x = \pi$

Table 2.15: Position of line nodes protected by nonsymmorphic symmetry, based on the Fermi surfaces in Fig. 2.2.

order to study this situation, we made a calculation in the presence of the line nodes, and ob-

⁷It is true that $(0\bar{1}1)$ or $(01\bar{1})$ surface should be chosen to preserve G_x . However, we can consider an alternative glide symmetry $G'_x = \{ E \mid m\mathbf{a} - n\mathbf{b} \} G_x$ with $(m, n) \in \mathbb{Z}^2$, which have the same glide topological invariants. Thus, topological surface states corresponding to G_x appear on all the surface directions of the form $(0, 2n+1, 2m+1)$. It would be possible to choose a surface direction to avoid the overlap of point nodes with zero-energy surface states.

tained Fig. 2.7. The panel (a) shows the surface states of A_u symmetry with the parameters

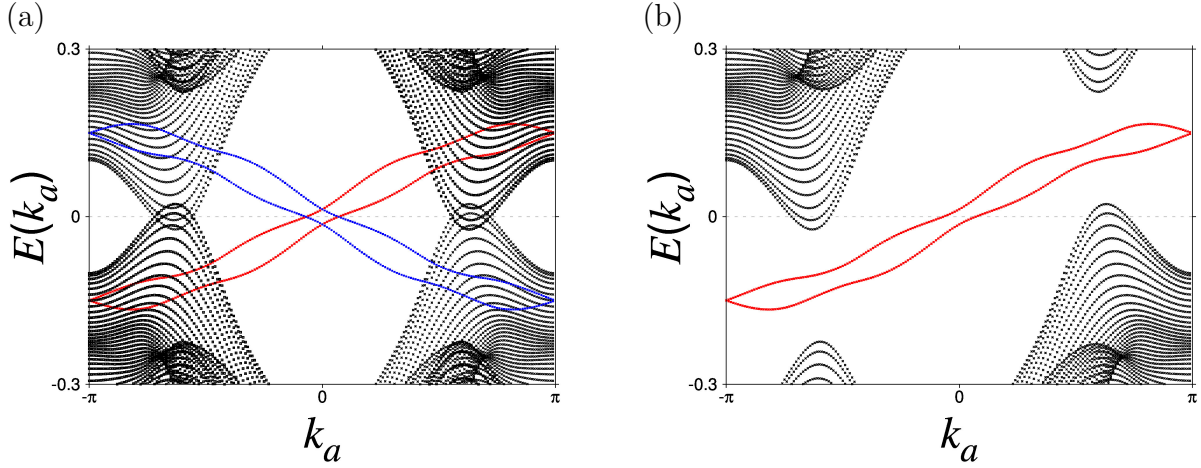


Figure 2.7: $\mathbb{Z}_4$ surface states in the presence of the line nodes protected by nonsymmorphic symmetry. The panel (a) shows the full spectrum, while the panel (b) shows the energy eigenvalues with positive glide eigenvalue.

same as the panel (a) of Fig. 2.5, with retaking $\epsilon_1 \rightarrow 5\epsilon_1$ in Eq. (2.6.10). The bulk energy states highlighted with black cross the zero energy, and thus there appear line nodes. In the panel (b), we showed energy eigenstates within positive glide eigensector. Importantly, band gap opens within the glide eigensector, and the spectrum is like a topological semimetal state. The presence of the band gap owing to finite interband gap function is a general feature of the line nodes protected by nonsymmorphic symmetry, where only intraband component of the gap function is prohibited. Therefore, we can define $\mathbb{Z}_4$ invariant by taking the ‘curved chemical potential’, to keep the contribution from the valence bands, and reproduce the values in Table 2.11. Note that bulk states and surface states do not mix with each other in the panel (a), since they have different glide eigenvalues. Thus, $\mathbb{Z}_4$ topological invariants and corresponding surface states are robust against the presence of line nodes protected by nonsymmorphic symmetry.

Furthermore, we note that the diameter of the line nodes may be small (or even absent) in UCoGe. As has been clarified in Ref. [110], spin-orbit splitting of the Fermi surfaces is indispensable to obtain stable line nodes protected by nonsymmorphic symmetry: The line nodes are gapped out when the splitting of the Fermi surfaces is smaller than or comparable to the strength of the order parameter. In the Fermi surfaces of Ref. [9, 10], the splitting of Fermi surfaces is small especially for $k_y = \pi$. The splitting is roughly estimated to be ~ 0.01 eV from Ref. [9].⁸ This energy scale is renormalized due to electron correlation by a

⁸In Fig. 4(b) of Ref. [9], half the ticks of the figure is 0.1 eV, and the splitting of the cylinder Fermi surfaces around X point is hardly visible in this energy scale. We adopt the splitting ~ 0.01 eV as a largest estimate.

factor $1/z \lesssim 100$, which we assume as a typical value of heavy-fermion compounds. Then, we obtain the splitting ~ 0.1 meV, which is smaller than the magnitude of the gap function expected from the transition temperature $T_c = 0.5$ K. Thus, line nodes might be absent, or, even in their presence, their size is expected to be small in the Brillouin zone (as in Fig. 2.7). This makes UCoGe as a good platform to observe $\mathbb{Z}_4$ surface states.

2.7.3 Possibility and influence of deviation of Fermi surfaces

We should discuss the possibility that the Fermi surfaces obtained by first-principles calculation [9, 10] deviate from the true Fermi surfaces of UCoGe, because first-principles calculation might be inaccurate for heavy-fermion systems. Indeed, with a method different from Ref. [9, 10] applied, first-principles calculation predicted Fermi surfaces with different topology [11]: The cylinder Fermi surfaces given in Ref. [10, 10] are changed to electron pockets around S point. Accordingly, $\nu_{\pm}^{(z)}(\pi)$ vanishes due to the absence of Fermi surfaces on the $S - R$ line, while the other topological invariants remain the same (Table 2.16). Im-

IR	Topological invariants	
	G_z	G_x
A_u	$\theta_4^{(z)}(\pi) = 2$	$\theta_4^{(x)}(\pi) = 2$
B_{1u}	$\theta_4^{(z)}(\pi) = 2$	$\nu_{\pm}^{(x)}(\pi) = 1$
B_{2u}	$\nu_{\pm}^{(z)}(\pi) = 0$	$\nu_{\pm}^{(x)}(\pi) = 1$
B_{3u}	$\nu_{\pm}^{(z)}(\pi) = 0$	$\theta_4^{(x)}(\pi) = 2$

Table 2.16: Glide topological invariants evaluated for the Fermi surfaces of Ref. [11].

portantly, $\mathbb{Z}_4$ invariant $\theta_4^{(z)}(\pi)$ is still nontrivial in this case, meaning that the formula of $\theta_4^{(z)}(\pi)$ in Table 2.8 is not applicable in this case, due to the strong effective spin-orbit coupling. Nontrivial $\mathbb{Z}_4$ invariants are correctly obtained from the formulas in Table 2.7, with $M^{\text{occ.}}(U) = 252 \in 8\mathbb{Z} + 4$ from Ref. [11]. In summary, we obtain $\mathbb{Z}_4$ topological superconductivity also in this case.

To be precise, it must be noted that the first-principles calculations [9, 10, 11] are done for the paramagnetic normal state at the ambient pressure. Since our focus is on the paramagnetic normal state at high pressure, pressure effect on the calculated Fermi surfaces should be discussed. According to the first principles calculation [120] with using the lattice constants measured under pressure [121], it has been shown that Fermi surface structure hardly changes by applying pressure, and accordingly, topological invariants are unaffected. The effect of electron correlation, which is not included in the calculations, should also be

The splitting on the $k_y = \pi$ plane seems to be of the same order, by looking at the Fermi surfaces in Fig. 4 of Ref. [9].

discussed. However, we expect that correlation effect may be small, because interaction is relatively suppressed under pressure. Thus, it would be natural to expect that the Fermi surfaces obtained by Refs. [9, 10, 11] capture essential features of the true Fermi surfaces under pressure.

Experimentally, Fermi surfaces of UCoGe (both in the ferromagnetic and paramagnetic states) have not yet been clarified. Angle-resolved photoemission spectroscopy (ARPES) experiment has been performed in the paramagnetic state at ambient pressure, but the results are hardly visible near the Fermi energy [9, 10]. Another attempt is the Quantum oscillation measurements, which have been done at ambient pressure for magnetic field around b -axis and c -axis [122, 123]. Small Fermi pockets were observed for small magnetic field regime, accompanied by successive Lifshitz transitions under higher fields [123]. The authors of Ref. [123] argue that the observed small Fermi pockets may correspond to the cylinder or spherical Fermi surfaces around S point obtained in Refs. [9, 10, 11], while the results are totally inconsistent with the calculated Fermi surfaces for the Ferromagnetic state obtained in Ref. [11] (this might be natural, since the calculated ferromagnetic moment $0.47\mu_B/U$ [11] is one order of magnitude larger than the experimental value $0.06\mu_B/U$ [54], and the band structure seems to be sensitive to the strength of Zeeman field). Since the S Fermi surfaces are essential for topological superconductivity, further study is awaited to validate this proposal. In particular, quantum oscillation measurements under pressure is desirable, to unambiguously determine Fermi surfaces for the paramagnetic state.

2.7.4 Toward the experimental identification of $\mathbb{Z}_4$ topological superconductivity

Here, we briefly discuss experiments to identify topological superconductivity in UCoGe. First of all, the determination of Fermi surfaces and pairing symmetry is highly desired for an experimental identification of UCoGe as topological glide superconductivity. Even when the true Fermi surfaces deviate from those given in Ref. [9, 10], we can easily obtain the corresponding topological invariants by our Fermi-surface formulas. Thus, topological superconductivity can be identified through these bulk properties.

One of the direct approaches to identify topological superconductivity is to use surface probes, such as ARPES. Unfortunately, such an experiment is difficult to be done in this case, since time-reversal symmetric superconductivity is realized under pressure with low temperatures. A possible route to observe gapless surface quasiparticles is to measure magnetic properties of the surfaces as well as their dependence on field direction. Surface magnetic susceptibility is expected to be strongly dependent on field direction, because zero energy eigenstates of $\theta_4(\pi) = 2$ states hybridize with each other only for field direction breaking the relevant glide symmetry. A feasible measurement might be NMR, which has recently detected nanoscale magnetic properties [124].

Another strategy is to search for a material showing time-reversal symmetric superconductivity at ambient pressure, which enables us to use surface probes. In this direction, we refer to CrAs family as a promising platform: CrAs and CrP crystalize in the space group $Pnma$, and have cylinder Fermi surfaces around S point, as in UCoGe [125]. Thus, our formulas also predict $\mathbb{Z}_4$ and/or $\mathbb{Z}_2$ topological superconductivity for these systems by Table 2.12, when odd-parity superconductivity is realized. Interestingly, paramagnetic superconductivity is realized in CrAs by applying pressure or substituting P for As [126, 127], and there is an experimental suggestion of odd-parity superconductivity by field-angle dependence of upper critical field [128], along with the absence of the coherence peak reported by NQR [129]. Further study on the nature of the paramagnetic superconducting phase in these systems is an interesting future issue.

2.8 Summary

In this chapter, we investigated time-reversal symmetric topological glide superconductivity specified by $\mathbb{Z}_4$ and/or $\mathbb{Z}_2$ topological invariants, focusing on the high-pressure superconducting phase of UCoGe. Formulas connecting glide topological invariants with symmetry indicators are derived, and are further simplified for the space group $Pnma$, clarifying that the topology is determined by the occupation number at high-symmetry points and the number of Fermi surfaces. Combining the formulas with previously obtained first-principles calculations of UCoGe, we showed that all the Brillouin-zone-face topological invariants take nontrivial values. Thus, UCoGe under pressure is identified as a promising candidate of topological glide superconductivity. In particular, three out of four pairing symmetries are $\mathbb{Z}_4$ nontrivial topological glide superconductivity, which has never been proposed for real superconductors. We also propose CrAs and related materials as another promising platform of $\mathbb{Z}_4$ topological glide superconductivity.

Chapter 3

Chirality polarizations and spectral bulk-boundary correspondence

Bulk-boundary correspondence (BBC) is the central concept in the study of topological materials [22]. It has been clarified that nontrivial topological invariants defined in the bulk predict the number of gapless surface states. BBC predicts surface spin currents and Majorana zero modes in topological insulators and superconductors, respectively [16, 18, 130]. Thus, BBC is important from both fundamental and practical points of view.

We point out that there is another context where surface physics is dominated by the bulk, as is the case for BBC. Electric polarization, that is the surface electric charge, is known to be a bulk property modulo a polarization quantum [131, 132, 133, 134]. This is a remarkable result, since surface electric charge is apparently sensitive to the surface details. It has also been established that the orbital magnetic moment, which is given by $\langle \hat{x}\hat{j}_y - \hat{y}\hat{j}_x \rangle / 2L^2$ in 2D, is a bulk property [134, 135, 136, 137]. We would say these facts may be regarded as a kind of BBC, in the sense that apparently surface sensitive quantities are actually a bulk property.

In contrast to electric and magnetic dipole moments, quantum-mechanical formulation of higher order multipole moments are still under progress. For example, electric quadrupole and octupole moments are shown to be the bulk property in the presence of certain crystalline symmetries [66, 67]. However, whether they are the bulk property in the absence of the symmetries is still an ongoing problem [138, 139, 140]. There is also an attempt to define spin magnetic quadrupole moments. However, resultant expressions are gauge dependent [141, 142], implying they may not be bulk properties. Magnetic quadrupole moments have also been studied by local thermodynamics, and gauge-invariant expressions are obtained [143, 144, 145, 146]. However, it is not clarified that the formulation based on the local thermodynamics is equivalent with the magnetic multipole moments defined in classical electromagnetism [147]. Multipole moments are among the most fundamental physical quantities, and thus the formulation which allows their quantitative evaluation is one of the most

important issues of condensed matter physics. Therefore, it is necessary to gain deeper insight into for what physical quantities ‘BBC’ holds, to clarify the physical nature of multipole moments.

Recently, Tamura *et al.* proposed an interesting relation satisfied in one-dimensional chiral symmetric systems [14]. In the *spectral bulk-boundary correspondence* (SBBC) dubbed by the authors, a component of Green’s function spatially integrated around the surface is, surprisingly, a bulk property, and the correspondence is robust against surface disorders. In the context of superconductivity, spectral bulk-boundary correspondence predicts as a bulk property surface accumulation of odd-frequency Cooper pairs, which play important roles in the physics of heterostructures and Josephson junctions [17, 148, 149]. In particular, zero-frequency limit reproduces the topological bulk-boundary correspondence of one-dimensional chiral symmetric systems [63, 150, 151], and thus SBBC is regarded as a generalization of the concept of bulk-boundary correspondence into finite frequencies.

SBBC is an interesting relation: Presence and absence of surface odd-frequency Cooper pairs are the bulk property, which is contrary to the intuition. In addition, it might be practically useful, since it may give a kind of sum rule, for example to Green’s function calculated with quasiclassical theories. However, the original proposal of SBBC [14] was the conjecture based on the observation for specific models, and there has not been a formal proof.

In this chapter, we present a proof of SBBC based on the analogy with electric polarization [4]. We give two proofs: one is via Wannier functions, while the other is via adiabatic deformation of Hamiltonian. This chapter is constructed as follows. In Sec. 3.1, we show the statement of SBBC, and point to the similarity to electric polarization. In Sec. 3.2, we briefly review the derivation of electric polarization [131, 132, 133, 134], focusing on the microscopic excess charge accumulated around the surface related to the intercellular Zak phase [152]. In Sec. 3.3, we prove SBBC based on the analogy with electric polarization. We establish that charge neutrality conditions and equation of continuity are satisfied for chirality charge, and give proofs based on them. In Sec. 3.5, we make a comment on the spin magnetic quadrupole moments, or the spin density polarization, where similar formalism predicted gauge-dependent results [141]. The results for electric, spin density, and chirality polarizations are compared with each other. In Sec. 3.6, we summarize the essence of the derivation and make some discussion.

3.1 Statement of spectral bulk-boundary correspondence

In this section, we present the statement of SBBC [14]. Let us consider an one-dimensional system with chiral symmetry represented by the chiral operator $\hat{\Gamma}$ satisfying $\{\hat{\Gamma}, \hat{H}\} = 0$. SBBC claims an equality holds between the two quantities $zF(z)$ and $w(z)$ defined in open

and periodic boundary conditions, respectively:

$$zF(z) = w(z). \quad (3.1.1)$$

Here, z is a complex-valued variable corresponding to frequency, which takes the values except for the energy eigenstates on the real axis.

The quantity $F(z)$ is defined in open-boundary condition with the system spreading over $0 \leq x < N$ as

$$F(z) = \int_{N_c}^N dx \text{Tr}[\hat{n}(x)\hat{\Gamma}\hat{G}(z)] \quad (N_c \gg 1). \quad (3.1.2)$$

Here, $N_c \in \mathbb{N}$ with $0 < N_c/N < 1$ is the cut-off unit cell deep inside the bulk (lattice constant is set to unity); for example, we can set $N_c = N/2$. $\hat{G}(z) = (z - \hat{H})^{-1}$ is the Green function with Hamiltonian $\hat{H}$ (corresponding to $\hat{H}^{(1)}$ in Sec. 1.3.3) in the open-boundary condition, while $\hat{n}(x)$ is the particle density operator ¹

$$\hat{n}(x) = \sum_l |x, l\rangle \langle x, l|. \quad (3.1.3)$$

The expression Eq. (3.1.2) is equivalent with the component of Green's function proportional to Γ accumulated around the right end of the system. For the case of superconductors, Γ is off-diagonal in the Nambu space, and therefore $F(z)$ corresponds to a component of anomalous Green's function. Furthermore, $F(z)$ is odd in frequency, as is clear from $[\hat{n}(x), \hat{\Gamma}] = 0$ and $\hat{\Gamma}\hat{G}(z) = -\hat{G}(-z)\hat{\Gamma}$:

$$F(-z) = -F(z). \quad (3.1.4)$$

Thus, $F(z)$ is interpreted as the surface accumulation of odd-frequency Cooper pairs.

The quantity $w(z)$ is defined in periodic boundary conditions as

$$w(z) = - \int_{-\pi}^{\pi} \frac{dk}{4\pi i} \text{tr}[\Gamma G_k(z) \partial_k G_k^{-1}(z)], \quad (3.1.5)$$

with $G_k(z) = (z - H_k)^{-1}$ and H_k the Bloch Hamiltonian in the periodic basis (see Eq. (1.3.29)). Here, the small trace “tr” is the trace for the internal degrees of freedom in the wave-number space, e.g. $\text{tr}[H_{\mathbf{k}}] = \sum_{\alpha} [H_{\mathbf{k}}]_{\alpha\alpha}$, in contrast to the large trace “Tr” taken for the whole Hilbert space, e.g. $\text{Tr}[\hat{O}] = \sum_{\mathbf{k}} \sum_{\alpha} \langle \mathbf{k}, \alpha | \hat{O} | \mathbf{k}, \alpha \rangle$. Note that the presence or absence of the hat correspond to the operator on the Hilbert space or just a matrix, respectively. For example, $H_{\mathbf{k}}$ is a matrix corresponding to the operator $\hat{H}_{\mathbf{k}}$ (for the details of notations, see Sec. 1.3). Importantly, $w(0)$ coincides with the usual topological winding number for chiral symmetric systems [63, 150, 151]. For this reason, $w(z)$ may be regarded as a generalization of the winding number into complex frequencies, and is named as the generalized winding number.

¹Formally, we consider a chiral symmetric insulator. Superconductors can also be described based on this setup, by regarding BdG Hamiltonian as Bloch Hamiltonian of an insulator.

Our idea of the proof is the analogy with electric polarization. Let us define z -dependent chirality charge $\rho_\Gamma(z, x)$ by

$$\rho_\Gamma(z, x) = \text{Tr}[\hat{n}(x)\hat{\Gamma}\hat{G}(z)]. \quad (3.1.6)$$

Then, $F(z)$ is clarified to be nothing but the accumulated surface chirality charge

$$F(z) = \int_{N_c}^N dx \rho_\Gamma(z, x). \quad (3.1.7)$$

On the other hand, $w(z)$ includes Γ as well as a derivative of k which roughly corresponds to the position operator $\hat{R}$. Thus, $w(z)$ would be something like polarization of chirality $\sim \langle \Gamma \hat{R} \rangle$, which seems to be closely related to $F(z)$. Thus, it is natural to expect that SBBC can be shown by a discussion parallel to the derivation of electric polarization. Below, we review electric polarization and then prove SBBC in two ways analogous to electric polarization.

3.2 Short review of electric polarization

In this section, we make a review of the derivation of the Berry phase formula for the surface charge [131, 132, 133, 134, 152]. In particular, we focus only on the derivation of the intercellular Zak phase formula [152], which is shown to be directly related to SBBC.

Let us consider an one-dimensional band insulator spreading over $0 \leq x < N$ with N the total number of unit cells (lattice constant is set to unity). For a while, we adopt open boundary condition, and assume that the occupied electron states are spanned by the generalized Wannier functions (GWFs) $\{|W_\mu(R)\rangle\}_{R,\mu}$, following [132, 134]. GWFs are the open-boundary-condition counterpart of the Wannier functions $\{|w_\mu(R)\rangle\}_{R,\mu}$, which are the localized basis of occupied electron states in periodic boundary condition. There are $\sum_\mu 1$ electron states assigned to each unit cell specified by $R \in \mathbb{Z}$. GWFs are assumed to be localized in the same way as the genuine Wannier functions, and to coincide with the genuine Wannier functions as R getting away from the surface. The presence of such GWFs is proven at least for the case of inversion symmetric systems without spin-orbit coupling [153, 154, 155]. In this section, we assume for simplicity that the bands are isolated in periodic boundary condition. Thus, genuine Wannier functions are given by just the Fourier transform of the energy eigenstates:

$$|w_\mu(R)\rangle = \frac{1}{\sqrt{N}} \sum_R e^{-ikR} |\psi_\mu(k)\rangle. \quad (3.2.1)$$

For simplicity, ions are assumed to be a uniform background positive charge ensuring the total charge neutrality of the system, which is essential for the origin-independence of electric polarization [147]. Thus, charge density is given by the sum of the two contributions,

$$\rho(x) = \rho_{\text{el}}(x) + \rho_{\text{ion}}(x), \quad (3.2.2a)$$

$$\rho_{\text{el}}(x) = \sum_{R,l,\mu} |\langle x, l | W_\mu(R) \rangle|^2, \quad \rho_{\text{ion}}(x) = - \sum_\mu 1, \quad (3.2.2b)$$

with electron charge set to unity.

3.2.1 Equivalence of surface charge with polarization

In the following, we derive the intercellular Zak phase formula [152] for the surface excess charge

$$Q = \int_{N_c}^N dx \rho(x). \quad (3.2.3)$$

For this purpose, in this subsection, we rewrite Q to the form of electric polarization:

$$Q = \frac{1}{N} \sum_R \int_0^1 dr R \rho(R + r) + O(1/N). \quad (3.2.4)$$

This can be achieved by the following two steps.

First, let us rewrite Eq. (3.2.3) by averaged charge density:

$$\bar{\rho}(x) = \int_0^1 d[\Delta r] \rho(x + \Delta r). \quad (3.2.5)$$

The advantage to use $\bar{\rho}(x)$ is the charge neutrality within the unit cell:

$$\bar{\rho}(x) = 0. \quad (x \in \text{bulk}) \quad (3.2.6)$$

Actually, $\bar{\rho}(x)$ is the total charge in the unit cell, which must vanish. Note that $\bar{\rho}(x)$ is analogous to the coarse-grained charge density introduced in the classical electromagnetism [147], which also vanishes in uniform insulators, enabling us to use the discussion therein. We obtain

$$\sigma \equiv \int_{N_c-1}^N dx \bar{\rho}(x) \quad (3.2.7a)$$

$$= \int_{N_c-1}^N dx \int_0^1 dr \{ \partial_r (r \rho(x + r)) - r \partial_r \rho(x + r) \} \quad (3.2.7b)$$

$$= \int_{N_c}^{N+1} dx \rho(x) - \int_0^1 dr r \{ \rho(N + r) - \rho(N_c - 1 + r) \} \quad (3.2.7c)$$

$$= Q + \int_0^1 dr r \rho(N_c - 1 + r). \quad (3.2.7d)$$

Here, we used $\rho(x) = 0$ for $x \geq N$.

Next, we see that the coarse-grained surface charge σ is equivalent with the polarization of the system, as is known in electromagnetism [147]. We can rewrite σ as follows:

$$\sigma = \frac{1}{N} \int_{-1}^N dx x \bar{\rho}(x) + O(1/N), \quad (3.2.8)$$

since $\bar{\rho}(x)$ is finite only around $x \sim 0, N$ and damps rapidly in space elsewhere. Note that $\bar{\rho}(x)$ is finite for $x \geq -1$ by our definition of the average window. Furthermore, we obtain

$$\int_{-1}^N dx x \bar{\rho}(x) = \int_{-1}^N dx x \int_0^1 dr \rho(x+r) \quad (3.2.9a)$$

$$= \int_0^1 dr \int_{-1+r}^{N+r} dx (x-r) \rho(x) \quad (3.2.9b)$$

$$= \int_0^1 dr \int_{-1+r}^{N+r} dx x \rho(x) - \int_0^1 dr r \int_{-1+r}^{N+r} dx \rho(x) \quad (3.2.9c)$$

$$= \int_0^N dx x \rho(x) \quad (3.2.9d)$$

$$= \sum_R \int_0^1 dr (R+r) \rho(R+r). \quad (3.2.9e)$$

We used the total charge neutrality

$$\int_0^N dx \rho(x) = 0, \quad (3.2.10)$$

and $\rho(x) = 0$ outside the system, to obtain the fourth line. We also obtain

$$\int_0^1 dr r \rho(N_c - 1 + r) = \frac{1}{N} \sum_R \int_0^1 dr r \rho(R+r) + O(1/N), \quad (3.2.11)$$

by using the approximate translational invariance $\rho(R+r) \simeq \rho(R+1+r)$ for R in the bulk (the error of $\simeq$ is exponentially small). This completes the proof of Eq. (3.2.4).

Importantly, we used only the two charge neutrality conditions Eqs. (3.2.6) and (3.2.10) to show the equivalence of Eq. (3.2.3) with Eq. (3.2.4). This fact is quite important for the proof of SBBC.

3.2.2 Equivalence of surface excess charge with the intercellular Zak phase

Let us rewrite Q by wave-number-space quantities. By substituting the expression of $\rho(x)$, we obtain

$$Q = \frac{1}{N} \sum_{R,\mu} \langle W_\mu(R) | \hat{R} | W_\mu(R) \rangle - \frac{1}{N} \sum_{R,\mu} R \quad (3.2.12a)$$

$$= \frac{1}{N} \sum_{R,\mu} \langle W_\mu(R) | (\hat{R} - R) | W_\mu(R) \rangle. \quad (3.2.12b)$$

The second line is obtained as a consequence of the charge neutrality, and is important to move onto wave-number space. Indeed, owing to the localization of GWFs, the contribution

to Q comes from only the bulk lattice points, where $|W_\mu(R)\rangle$ coincides with $|w_\mu(R)\rangle$. Thus, we obtain the Zak phase formula for electric polarization,

$$Q = \frac{1}{N} \sum_{R,\mu} \langle w_\mu(R) | (\hat{R} - R) | w_\mu(R) \rangle \quad (3.2.13a)$$

$$= \sum_{\mu} \langle w_\mu(0) | \hat{R} | w_\mu(0) \rangle \quad (3.2.13b)$$

$$= i \sum_{\mu} \int \frac{dk}{2\pi} \langle u_{k,\mu} | \partial_k u_{k,\mu} \rangle. \quad (3.2.13c)$$

Here, it should be noted that the Zak phase formula for Q is written by the periodic part of Bloch functions in the periodic basis

$$|u_{k+2\pi,\mu}\rangle = |u_{k,\mu}\rangle = e^{-ik\hat{R}} |\psi_\mu(k)\rangle, \quad (3.2.14)$$

which is defined in Sec. 1.3. It should be noted that the well-known Berry phase formula [132, 134] for electric polarization p is given by

$$p = i \sum_{\mu} \int \frac{dk}{2\pi} \langle u_\mu(k) | \partial_k u_\mu(k) \rangle, \quad (3.2.15)$$

with $|u_\mu(k)\rangle = e^{-ik\hat{r}} |\psi_\mu(k)\rangle$. p coincides with the coarse-grained surface charge σ , not with Q [152].

3.3 Proof of SBBC based on Wannier functions

In this section, we present a proof based on Wannier functions. The derivation is parallel to that of intercellular Zak phase formula, owing to the neutrality conditions satisfied by the chirality charge.

3.3.1 Chirality charge neutrality

First of all, let us show the chirality charge neutrality conditions:

$$\int_0^N dx \rho_\Gamma(z, x) = 0, \quad \bar{\rho}_\Gamma(z, x) = 0 \quad (x \in \text{bulk}). \quad (3.3.1)$$

The total charge neutrality is shown as follows:

$$\int_0^N dx \rho_\Gamma(z, x) = \text{Tr}[\hat{\Gamma}\hat{G}(z)] \quad (3.3.2a)$$

$$= \frac{1}{z} \text{Tr}[\hat{P}_{E=0}\hat{\Gamma}] + \sum_{E \neq 0} \frac{\langle E | \Gamma | E \rangle}{z - E} \quad (3.3.2b)$$

$$= \frac{1}{z} \text{Tr}[(1 - \hat{P}_{E \neq 0})\hat{\Gamma}] \quad (3.3.2c)$$

$$= \frac{1}{z} \text{Tr}[\hat{\Gamma}]. \quad (3.3.2d)$$

Here, $\hat{P}_{E=0}$ and $\hat{P}_{E\neq 0}$ represent projection operator onto states with zero and finite energy, respectively, while the state $|E\rangle$ represents the eigenstate of Hamiltonian $\hat{H}$ with energy E in open boundary condition. Furthermore, $\text{Tr}[\hat{\Gamma}]$ should vanish.² Thus, the total chirality charge neutrality is satisfied.

The local charge neutrality in the bulk is shown as follows:

$$\bar{\rho}_\Gamma(z, x) = \int_0^1 dr \text{Tr}[\hat{n}(x+r)\hat{\Gamma}\hat{G}(z)] \quad (3.3.3a)$$

$$\simeq \int_0^1 dr \text{Tr}[\hat{n}(x+r)\hat{\Gamma}\hat{G}_{\text{PBC}}(z)] \quad (3.3.3b)$$

$$= \frac{1}{N} \sum_R \int_0^1 d[\Delta r] \text{Tr}[\hat{n}(x+R+\Delta r)\hat{\Gamma}\hat{G}_{\text{PBC}}(z)] \quad (3.3.3c)$$

$$= \frac{1}{N} \int_0^N dx \text{Tr}[\hat{n}(x)\hat{\Gamma}\hat{G}_{\text{PBC}}(z)] \quad (3.3.3d)$$

$$= \frac{1}{N} \text{Tr}[\hat{\Gamma}\hat{G}_{\text{PBC}}(z)] \quad (3.3.3e)$$

$$= 0. \quad (3.3.3f)$$

In the second line, we used the fact that the matrix element of the Green's function is replaced with that of periodic boundary condition, denoted as $\hat{G}_{\text{PBC}}(z)$, since $\hat{x}$ is a bulk point. Thus, we obtain the local chirality charge neutrality condition.

The two chirality charge neutrality conditions established above allows us to use the discussion in Sec. 3.2.1. Therefore, we obtain an equality for $F(z)$ analogous to Eq. (3.2.4):

$$F(z) = \frac{1}{N} \sum_R \int_0^1 d[\Delta r] R \rho_\Gamma(R + \Delta r, z) = \frac{1}{N} \text{Tr}[\hat{R}\hat{\Gamma}\hat{G}(z)]. \quad (3.3.4)$$

Here and hereafter, we neglect $O(1/N)$ contribution. This expression offers us a good start point to prove SBBC, as we see below.

3.3.2 Derivation of SBBC via Wannier functions

Let us prove SBBC based on the expression

$$zF(z) = \frac{z}{N} \text{Tr}[\hat{\Gamma}\hat{G}(z)\hat{R}]. \quad (3.3.5)$$

We can take the basis of Hilbert space as follows:

$$\langle |W_\mu(R)\rangle \rangle_{\mu,R} \oplus \langle \hat{\Gamma} |W_\mu(R)\rangle \rangle_{\mu,R} \oplus \langle |\phi_{\text{left}}\rangle \rangle \oplus \langle |\phi_{\text{right}}\rangle \rangle. \quad (3.3.6)$$

² According to the relation of chiral symmetry $\{\hat{\Gamma}, \hat{H}\} = 0$, the eigenvalues of $\hat{\Gamma}$ come with positive and negative pairs when Hamiltonian is invertible. Since $\hat{\Gamma}$ is independent of the parameters of $\hat{H}$, we may choose an atomic insulator, which is gapful, to show $\text{Tr}[\hat{\Gamma}] = 0$.

Here, $|\phi_{\text{left}}\rangle$ and $|\phi_{\text{right}}\rangle$ are, if any, the zero-energy boundary states on the left and right edge, respectively. The basis of the finite energy states are (assumed to be) spanned by GWFs for occupied states as well as their partner state in unoccupied states.³ First, the contribution to $zF(z)$ from the boundary states, denoted as $zF(z)|_{\text{surface}}$, is given by

$$zF(z)|_{\text{surface}} = \frac{1}{N} \left(\sum_{\text{right}} \langle \phi_{\text{right}} | \hat{\Gamma} \hat{R} | \phi_{\text{right}} \rangle + \sum_{\text{right}} \langle \phi_{\text{right}} | \hat{\Gamma} \hat{R} | \phi_{\text{right}} \rangle \right) \quad (3.3.7a)$$

$$= \sum_{\text{right}} \langle \phi_{\text{right}} | \hat{\Gamma} | \phi_{\text{right}} \rangle \quad (3.3.7b)$$

$$= w(0). \quad (3.3.7c)$$

The last line follows from the topological bulk-boundary correspondence [63, 150, 151], which states the equivalence of $w(0)$ with the eigenvalues of Γ possessed by the gapless surface states. Contribution from the other states, which we denote as $zF(z)|_{\text{bulk}}$, is given by

$$zF(z)|_{\text{bulk}} = \frac{2z}{N} \sum_{R,\mu} \langle W_\mu(R) | \hat{\Gamma} \hat{G}(z) \hat{R} | W_\mu(R) \rangle \quad (3.3.8a)$$

$$= \frac{2z}{N} \sum_{R,\mu} \langle W_\mu(R) | \hat{\Gamma} \hat{G}(z) (\hat{R} - R) | W_\mu(R) \rangle \quad (3.3.8b)$$

$$= \frac{2z}{N} \sum_{R,\mu} \langle w_\mu(R) | \hat{\Gamma} \hat{G}(z) (\hat{R} - R) | w_\mu(R) \rangle \quad (3.3.8c)$$

$$= 2z \sum_{\mu} \langle w_\mu(0) | \hat{\Gamma} \hat{G}(z) \hat{R} | w_\mu(0) \rangle \quad (3.3.8d)$$

$$= \frac{2zi}{N} \sum_{k,\mu} \langle u_{k,\mu} | \hat{\Gamma} \hat{G}_k(z) | \partial_k u_{k,\mu} \rangle \quad (3.3.8e)$$

$$= \frac{zi}{N} \sum_{k,\mu:\text{all}} \langle u_{k,\mu} | \hat{\Gamma} \hat{G}_k(z) | \partial_k u_{k,\mu} \rangle. \quad (3.3.8f)$$

The second line is obtained by the fact that $\hat{\Gamma} |W_\mu(R)\rangle$ belongs to the space of unoccupied states while $\hat{G}(z) |W_\mu(R)\rangle$ belongs to the space of occupied states. This is related to the local charge neutrality within a unit cell. In the last line, μ runs over both occupied and unoccupied bands.

In the following calculation, it is convenient to use matrix expression rather than opera-

³In the presence of the topological gapless end states, the number of GWFs assigned to unit cells near the surface might be smaller than $\sum_{\mu} 1$. However, this does not cause a problem, as is clear in the following discussion.

tors. Equation (3.3.8f) can be straightforwardly rewritten as

$$zF(z)|_{\text{bulk}} = \frac{zi}{N} \sum_{k,\mu:\text{all}} \mathbf{u}_{k,\mu}^\dagger \Gamma G_k(z) \partial_k \mathbf{u}_{k,\mu} \quad (3.3.9a)$$

$$= \frac{zi}{2N} \sum_k \text{tr} \left[\Gamma G_k(z) \sum_{\mu:\text{all}} \left(\partial_k \mathbf{u}_{k,\mu} \mathbf{u}_{k,\mu}^\dagger - \mathbf{u}_{k,\mu} \partial_k \mathbf{u}_{k,\mu}^\dagger \right) \right], \quad (3.3.9b)$$

with $G_k(z) = (z - H_k)^{-1}$. Since $zF(z)|_{\text{bulk}}$ is even in terms of z , we can symmetrize the right hand side. Thus, we obtain

$$zF(z)|_{\text{bulk}} = \frac{i}{2N} \sum_k \text{tr} \left[\Gamma \frac{z^2}{z^2 - H^2} \sum_{\mu:\text{all}} \left(\partial_k \mathbf{u}_{k,\mu} \mathbf{u}_{k,\mu}^\dagger - \mathbf{u}_{k,\mu} \partial_k \mathbf{u}_{k,\mu}^\dagger \right) \right] \quad (3.3.10a)$$

$$= -\frac{i}{2N} \sum_k \text{tr} \left[\Gamma \frac{z^2 H_k^{-1}}{z^2 - H_k^2} \sum_{\mu:\text{all}} \left(\partial_k \mathbf{u}_{k,\mu} \mathbf{u}_{k,\mu}^\dagger H_k + H_k \mathbf{u}_{k,\mu} \partial_k \mathbf{u}_{k,\mu}^\dagger \right) \right] \quad (3.3.10b)$$

$$= -\frac{i}{2N} \sum_k \text{tr} \left[\Gamma \frac{z^2 H_k^{-1}}{z^2 - H_k^2} \left(\partial_k H_k - \sum_{\mu:\text{all}} \partial_k \epsilon_\mu(k) \mathbf{u}_{k,\mu} \mathbf{u}_{k,\mu}^\dagger \right) \right] \quad (3.3.10c)$$

$$= -\frac{i}{2N} \sum_k \text{tr} \left[\Gamma \left(H_k^{-1} + \frac{H_k}{z^2 - H_k^2} \right) \partial_k H_k \right] \quad (3.3.10d)$$

$$= \int \frac{dk}{4\pi i} \text{tr} \left[\Gamma H_k^{-1} \partial_k H_k \right] - \int \frac{dk}{4\pi i} \text{tr} \left[\Gamma G_k(z) \partial_k G_k(z)^{-1} \right] \quad (3.3.10e)$$

$$= -w(0) + w(z). \quad (3.3.10f)$$

Finally, we conclude $zF(z) = zF(z)|_{\text{edge}} + zF(z)|_{\text{bulk}} = w(z)$. We note that it is also possible to show the equivalence of $zF(z)$ with $w(z)$ by considering their Laurent expansion and comparing the coefficients, as has been done in the original paper [4]. The derivation is essentially equivalent with the simplified proof adopted here.

It has been numerically reported that SBBC is extremely robust against surface disorder preserving chiral symmetry [14]. The reason for this robustness may be understood from the derivation presented above. Actually, surface disorder modulates only $O(1)$ number of GWFs around the surface out of $O(N)$ GWFs. Thus, the effect of the surface disorder is at most $O(1/N)$. In the next section, we clarify that SBBC holds more rigorously: The effect of surface disorder is exponentially small.

3.4 Proof of SBBC based on adiabatic deformation of Hamiltonian

The derivation of SBBC discussed in previous sections is based on some physical assumptions of GWFs. For this reason, we also show another route to obtain SBBC which is free of the

assumptions, although we believe the derivation in the previous section reasonable enough. In this section, we discuss a proof for continuum theory, instead of the proof for tight-binding models presented in Ref. [4]. The only difference is the expression of the equation of continuity, which has much simpler form in the continuum theory. Accordingly, the proof is also simplified, clarifying the essential role played by the equation of continuity.

The idea is again based on the analogy with electric polarization. A way to prove the equivalence of surface electric charge with the Berry phase is to consider the time evolution of the surface charge:

$$\frac{d}{dt} \int_{N_c}^N dx \rho(x) = \langle \hat{j}(N_c) \rangle, \quad (3.4.1)$$

with $\langle \cdot \rangle$ the expectation value of the ground state. This means that the rate of the change of the surface electric charge is given by the electric current $\hat{j}(x)$ flowing through the bulk region, which is, of course, a bulk property. Thus, the continuity equation is a key to prove the Berry phase formula for electric polarization.

In the following, we show that chirality charges also satisfy a kind of continuity equation for the adiabatic deformation of Hamiltonian. Let us consider z -dependent chirality charge $\rho_\Gamma(z, x)$, which has already been defined in Eq. (3.1.6) by

$$\rho_\Gamma(z, x) = \text{Tr}[\hat{n}(x)\hat{\Gamma}\hat{G}(z)]. \quad (3.4.2)$$

Suppose that Hamiltonian depends on a parameter λ as $\hat{H}_\lambda$. Then, we obtain

$$\partial_\lambda \rho_\Gamma(z, x) = \text{Tr}[\hat{n}(x)\hat{\Gamma}\hat{G}_\lambda(z)\partial_\lambda \hat{H}_\lambda \hat{G}_\lambda(z)] \quad (3.4.3a)$$

$$= \text{Tr}[[\hat{G}_\lambda(z), \hat{n}(x)]\hat{\Gamma}\hat{G}_\lambda(z)\partial_\lambda \hat{H}_\lambda] - \text{Tr}[\hat{n}(x)\hat{\Gamma}\hat{G}_\lambda(-z)\hat{G}_\lambda(z)\partial_\lambda \hat{H}_\lambda]. \quad (3.4.3b)$$

The second term has odd power of $\hat{H}_\lambda$ since $\hat{G}_\lambda(-z)\hat{G}_\lambda(z) = (\hat{H}_\lambda^2 - z^2)^{-1}$, and vanishes due to chiral symmetry. From $[\hat{G}_\lambda(z), \hat{n}(x)] = \hat{G}_\lambda(z)[\hat{H}_\lambda, \hat{n}(x)]\hat{G}_\lambda(z)$ and the charge conservation

$$\partial_x \hat{j}_\lambda(x) = -i[\hat{H}_\lambda, \hat{n}(x)] \quad (3.4.4)$$

with the current operator $\hat{j}_\lambda(x)$, we obtain

$$\partial_\lambda \rho_\Gamma(z, x) = i\partial_x \text{Tr}[\hat{G}_\lambda(z)\hat{j}_\lambda(x)\hat{G}_\lambda(z)\hat{\Gamma}\hat{G}_\lambda(z)\partial_\lambda \hat{H}_\lambda] \quad (3.4.5a)$$

$$\equiv -\partial_x j_\Gamma(z, x, \lambda). \quad (3.4.5b)$$

This equality means that the chirality charge is conserved during the adiabatic change of the Hamiltonian. It should be noted that the conservation law of chirality charge is not an operator identity, and that the chirality current locally vanishes when the Hamiltonian stays unchanged ($\partial_\lambda \hat{H}_\lambda = 0$). The first feature makes a clear contrast to the usual charge conservation law for the electric charge. Nevertheless, Eq. (3.4.5) enables us to relate the surface quantity $zF(z)$ with the bulk quantity $w(z)$, as we show in the following.

Our strategy of the proof is as follows. Let us consider an adiabatic deformation of the Hamiltonian

$$\hat{H}_\lambda = \hat{H}_0 + \lambda(\hat{H} - \hat{H}_0). \quad (3.4.6)$$

We assume that chiral symmetry is always preserved during the adiabatic deformation, $\{\hat{H}_\lambda, \hat{\Gamma}\} = 0$. First we show $z\partial_\lambda F(z) = \partial_\lambda w(z)$ for z away from the real axis. Next, we show $zF(z) = w(z)$ for $\hat{H}_0$, by choosing an atomic insulator, obtaining SBBC for z off the real axis. Finally, we extend the equality to the real axis around the origin by using analytic continuation.

Let us perform the spatial integration in $\partial_\lambda F(z)$:

$$\partial_\lambda F(z) = -j_\Gamma(z, N, \lambda) + j_\Gamma(z, N_c, \lambda) = j_\Gamma(z, N_c, \lambda). \quad (3.4.7)$$

The second equality follows from the open-boundary condition, which prohibits current flowing out of the system. Note that the right hand side is given by the matrix elements of the form

$$\langle x \sim N_c, l | \hat{G}_\lambda(z) \hat{\Gamma} \partial_\lambda \hat{G}_\lambda(z) | x \sim N_c, l' \rangle. \quad (3.4.8)$$

The effect of the surface can be neglected in these matrix elements, since Green's function damps exponentially in space with z off the real axis. Thus, we can replace the Green's function in open-boundary condition with that in periodic boundary condition. In the following, $\hat{G}$ and $\hat{H}$ represent quantity in periodic boundary condition.

Let us rewrite $\hat{j}_\lambda(N_c)$ in a form convenient for the discussion in periodic boundary condition. Owing to the translation symmetry of $\hat{H}$, we can replace $\hat{j}_\lambda(N_c)$ in $j_\Gamma(z, N_c, \lambda)$ with $\sum_R \hat{j}_\lambda(R)/N$. Furthermore, we obtain

$$\sum_R \hat{j}_\lambda(R) = - \sum_R \frac{\delta \hat{H}}{\delta A(R)} \quad (3.4.9a)$$

$$= - \sum_R \int_0^1 dr \frac{\delta \hat{H}}{\delta A(R+r)} - \int_0^1 dr r \sum_R \partial_r \frac{\delta \hat{H}}{\delta A(R+r)} \quad (3.4.9b)$$

$$= - \int dx \frac{\delta \hat{H}}{\delta A(x)} + i \int_0^1 d[\Delta r] \sum_R [\Delta r n(R + \Delta r), \hat{H}] \quad (3.4.9c)$$

$$= \partial_k [e^{-ik\hat{r}} \hat{H} e^{ik\hat{r}}]_{k \rightarrow 0} + i[\Delta \hat{r}, \hat{H}] \quad (3.4.9d)$$

$$= \partial_k [e^{-ik\hat{R}} \hat{H} e^{ik\hat{R}}]_{k \rightarrow 0}. \quad (3.4.9e)$$

This leads to the relation

$$e^{-ik\hat{R}} \left(\sum_R \hat{j}_\lambda(R) \right) e^{ik\hat{R}} = \partial_k \hat{H}_k, \quad (3.4.10)$$

for periodic boundary condition. By using energy eigenstates $|\psi_\mu(k)\rangle$, Green's function can be written as

$$\hat{G}_\lambda(z) = N \int \frac{dk}{2\pi} \sum_\mu \frac{|\psi_\mu(k)\rangle \langle \psi_\mu(k)|}{z - \epsilon_\mu(k)}. \quad (3.4.11)$$

Thus, $\partial_\lambda F(z)$ is given by, with $\hat{G}_{k,\lambda} = (z - \hat{H}_{k,\lambda})^{-1}$,

$$\partial_\lambda F(z) = -iN \int \frac{dk}{2\pi} \sum_\mu \frac{1}{z - \epsilon_\mu(k)} \langle \psi_\mu(k) | \hat{j}_\lambda(N_c) \hat{G}_\lambda(z) \hat{\Gamma} \hat{G}_\lambda(z) \partial_\lambda \hat{H}_\lambda | \psi_\mu(k) \rangle \quad (3.4.12a)$$

$$= -i \int \frac{dk}{2\pi} \sum_\mu \frac{1}{z - \epsilon_\mu(k)} \langle u_{k,\mu} | e^{-ik\hat{R}} \sum_R \hat{j}_\lambda(R) e^{ik\hat{R}} \hat{G}_{k,\lambda}(z) \hat{\Gamma} \hat{G}_{k,\lambda}(z) \partial_\lambda \hat{H}_{k,\lambda} | u_{k,\mu} \rangle \quad (3.4.12b)$$

$$= -i \int \frac{dk}{2\pi} \sum_\mu \frac{1}{z - \epsilon_\mu(k)} \langle u_{k,\mu} | \partial_k \hat{H}_{k,\lambda} \hat{G}_{k,\lambda}(z) \hat{\Gamma} \hat{G}_{k,\lambda}(z) \partial_\lambda \hat{H}_{k,\lambda} | u_{k,\mu} \rangle \quad (3.4.12c)$$

$$= \int \frac{dk}{2\pi i} \text{tr} [G_{k,\lambda} \partial_k H_{k,\lambda} G_{k,\lambda}(z) \Gamma G_{k,\lambda}(z) \partial_\lambda H_{k,\lambda}]. \quad (3.4.12d)$$

This can be rewritten in the form of generalized winding number as follows. We use the following identities:

$$\text{tr} \left[\Gamma \frac{H_{k\lambda}}{z^2 - H_{k\lambda}^2} \partial_i H_{k\lambda} \frac{z}{z^2 - H_{k\lambda}^2} \partial_j H_{k\lambda} \right] = 0, \quad (3.4.13a)$$

$$\epsilon_{ij} \text{tr} \left[\Gamma \frac{H_{k\lambda}}{z^2 - H_{k\lambda}^2} \partial_i H_{k\lambda} \frac{H_{k\lambda}}{z^2 - H_{k\lambda}^2} \partial_j H_{k\lambda} \right] = 0, \quad (3.4.13b)$$

where i, j take either λ or k , and ϵ_{ij} is an antisymmetric tensor satisfying $\epsilon_{\lambda k} = 1$. We obtain

$$\partial_\lambda z F_\lambda(z) = z \int \frac{dk}{2\pi i} \text{tr} \left[\partial_k H_{k\lambda} \Gamma \frac{1}{z^2 - H_{k\lambda}^2} \partial_\lambda H_{k\lambda} \frac{z + H_{k\lambda}}{z^2 - H_{k\lambda}^2} \right] \quad (3.4.14a)$$

$$= \frac{\epsilon_{ij}}{2} \int \frac{dk}{2\pi i} \text{tr} \left[\Gamma \frac{z}{z^2 - H_{k\lambda}^2} \partial_i H_{k\lambda} \frac{z}{z^2 - H_{k\lambda}^2} \partial_j H_{k\lambda} \right] \quad (3.4.14b)$$

$$= \frac{\epsilon_{ij}}{2} \int \frac{dk}{2\pi i} \text{tr} \left[\Gamma \frac{z + H_{k,\lambda}}{z^2 - H_{k\lambda}^2} \partial_i H_{k\lambda} \frac{z + H_{k,\lambda}}{z^2 - H_{k\lambda}^2} \partial_j H_{k\lambda} \right] \quad (3.4.14c)$$

$$= \frac{\epsilon_{ij}}{2} \int \frac{dk}{2\pi i} \text{tr} [\Gamma G_{k,\lambda} \partial_i H_{k\lambda} G_{k,\lambda} \partial_j H_{k\lambda}] \quad (3.4.14d)$$

$$= -\frac{\epsilon_{ij}}{2} \int \frac{dk}{2\pi i} \text{tr} [\Gamma \partial_i G_{k,\lambda} \partial_j G_{k\lambda}^{-1}] \quad (3.4.14e)$$

$$= \partial_\lambda w(z). \quad (3.4.14f)$$

This equality holds even right on topological phase transition points, since we are considering $\text{Im } z \neq 0$.

Next, let us consider an atomic insulator $\hat{H}_0$. In particular, we choose

$$\langle R + \Delta r, l | \hat{H}_0 | R' + \Delta r', l' \rangle = h_0 \delta_{R,R'} (\sigma_z \otimes 1)_{(\Delta r, l), (\Delta r', l')} \quad (3.4.15)$$

by retaking the basis of internal degrees of freedom so as to satisfy

$$\langle R + \Delta r, l | \hat{\Gamma} | R' + \Delta r', l' \rangle = \delta_{R,R'} (\sigma_x \otimes u)_{(\Delta r, l), (\Delta r', l')} \quad (3.4.16)$$

with u some unitary matrix. In this case, we explicitly obtain

$$F(z) \propto \text{tr} \left[\sigma_x \begin{pmatrix} 1/(z - h_0) & 0 \\ 0 & 1/(z + h_0) \end{pmatrix} \right] = 0. \quad (3.4.17)$$

We also obtain $w(z) = 0$ since $\partial_k H_k = 0$. Thus, we obtain SBBC for $\text{Im } z \neq 0$.

Finally, let us extend the obtained relation to $z \sim 0$. This can be achieved by an analytic continuation. By expanding energy eigenstates, $zF(z)$ is written as

$$zF(z) = \int_{N_c}^N dx \sum_E \frac{z \langle E | \hat{n}(x) \hat{\Gamma} | E \rangle}{z - E}. \quad (3.4.18)$$

This is analytic around the origin as well as $\text{Im } z \neq 0$. On the other hand, $w(z)$ is written as

$$w(z) = \int_{-\pi}^{\pi} \frac{dk}{4\pi i} \sum_{\mu} \frac{\mathbf{u}_{k,\mu}^{\dagger} \Gamma \partial_k H_k \mathbf{u}_{k,\mu}}{z - \epsilon_{\mu}(k)}. \quad (3.4.19)$$

This is also analytic around the origin and $\text{Im } z \neq 0$, since the system is gapful for periodic boundary condition. Thus, $zF(z)$ and $w(z)$ coincide with each other even around $z \sim 0$ according to the uniqueness of analytic continuation. This completes the proof of SBBC. We also note that the proof presented in this section includes a fully quantum-mechanical proof of topological bulk-boundary correspondence in chiral symmetric one-dimensional system.

Before closing this section, we evaluate the effect of surface disorder on SBBC. In the process of the derivation above, the effect of surface disorder (preserving chiral symmetry) may appear only in the matrix element of the form (3.4.8). However, the dependence of such bulk matrix elements of Green's function on surface Hamiltonian is only of the order $e^{-|N - N_c|/\xi}$ with some length scale ξ , which is negligible. This explains the reported robustness of SBBC [14].

3.5 Discussion

In previous sections, we have shown that SBBC can be regarded as the polarization of chirality, and thereby proved it. In particular, one of the proofs is based on the Wannier-function formalism. In this section, we make a comment on the formulation of spin magnetic quadrupole moment, or *spin density polarization* $\text{Tr}[\hat{s}_i \hat{x}_j \theta(-\hat{H})]$ with $\theta(x)$ the heaviside step function, based on Wannier functions [141], where gauge-dependent expressions have been reported. The result makes a clear contrast to the gauge-independent formula of chirality polarization. It is important to clarify why gauge-dependent and independent results are obtained for spin density and chirality polarizations, respectively, since the methods used are common. In the following, we discuss the conditions for ‘bulk-boundary correspondence’

of polarizations, by comparing the similarities and differences between electric, spin density, and chirality polarizations.

For simplicity, let us consider 1D systems to discuss spin density polarization. Rewriting the definition by using GWFs, we obtain

$$\text{Tr}[\hat{s}_i \hat{x} \theta(-\hat{H})] = \sum_{R,\mu} \langle W_\mu(R) | \hat{s}_i (\hat{x} - R) | W_\mu(R) \rangle + \sum_{R,\mu} R \langle W_\mu(R) | s_i | W_\mu(R) \rangle. \quad (3.5.1)$$

The authors of Ref. [141] claim that the second term vanishes except in ferromagnets and ferrimagnets and can be ignored. However, we would say this is not correct, since finite magnetic moment can exist around the surface even in antiferromagnets. Furthermore, it can be shown that the second term can change by an arbitrary small value when the basis set of GWFs is retaken. (These points are exemplified in the next subsection.) Since the left hand side is independent of the choice of GWFs, this fact means that the first term is also dependent on the choice of GWFs, naturally leading to gauge dependence of the corresponding wave-number space expression. Once contribution from the surface GWFs is correctly included, if possible, spin density polarization may have a well-defined wave-number space expression, as is the case for orbital magnetic moments [135].

Next, let us discuss electric polarization. In particular, let us reconsider the derivation of Q . In this case, the $\hat{s}_i \hat{x}$ in first term is replaced with $\hat{R}$, while the second term of Eq. (3.5.1) is replaced with $\sum_{R,\mu} R$, which is independent of the basis choice of GWFs (though is origin dependent, and should be cancelled out with ion charge). Thus, we can safely pass to wave-number space with using Wannier functions assigned to each unit cell *in the same manner* as GWFs, which corresponds to a specific gauge fixing of Wannier functions. Such a gauge associated with Q in open boundary condition is sensitive to the surface details, and thus indeterminable only from the bulk information. However, non-integral part of Eqs. (3.2.13b) and (3.2.13c) is gauge-independent, and thus can be calculated with arbitrary gauge choice. This is why the replacement of $|W_\mu(R)\rangle$ with $|w_\mu(R)\rangle$ defined in Eq. (3.2.1) predicts the correct value modulo a quantum. Note that the same thing can be said about the spin density polarization in collinear magnets in the absence of spin-orbit coupling, because we can make the same discussion for each spin species. Thus, polarization of the charges corresponding to local symmetries (such as SU(2) symmetry) are bulk properties modulo polarization quantum.

Finally, as for chirality polarizations, the second term of Eq. (3.5.1) completely vanishes owing to chiral symmetry. Furthermore, the first term is gauge-invariant, since it includes only interband components of the position operator. This is why we obtained completely gauge-invariant expression of chirality polarizations. Note that these properties originate from the chiral symmetry, that is, local antisymmetries. Thus, we can say that polarizations of the charges corresponding to local antisymmetries are bulk properties. It should be noted that local antisymmetry ensures a component of *Green's function* to be a bulk property, while local symmetry ensures only the polarization, a *scalar quantity*. In this sense, local

antisymmetries impose stronger constraints on the surface physics than local symmetries. The strong constraints by the bulk are especially important for time-reversal symmetric superconductivity, where various antisymmetries may intrinsically emerge in combination with crystalline symmetries.

3.5.1 Illustration of the gauge dependence of spin density polarization

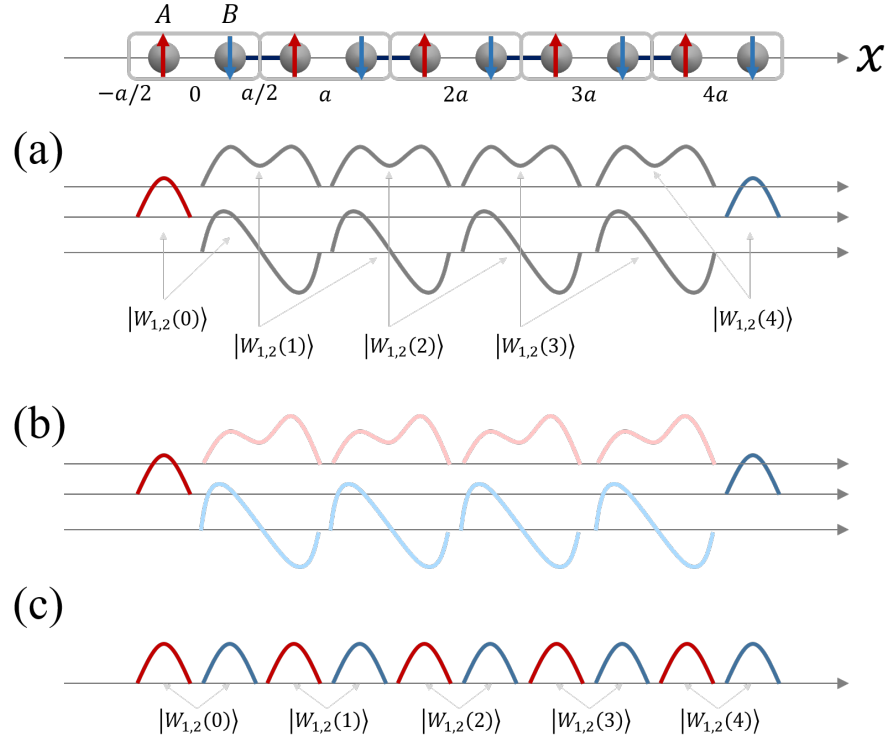


Figure 3.1: Schematic picture of the model $\hat{H}_+$ for $N = 5$ and possible choice of GWFs. The size of a unit cell a is set to unity.

Here, we illustrate the dependence of spin density polarization on the choice of GWFs. Let us consider an spin-orbit coupled antiferromagnetic chain described by the Hamiltonian

$$\hat{H} = \sum_{R=0}^{N-1} \mathbf{c}_R^\dagger (-h\sigma_z s_z - \xi\alpha\sigma_y s_x) \mathbf{c}_R + \left(\sum_{R=0}^{N-2} \mathbf{c}_R^\dagger (i\alpha s_x \sigma_-) \mathbf{c}_{R+1} + h.c. \right). \quad (3.5.2)$$

Here, $\mathbf{c}_R^\dagger = (c_\uparrow^\dagger(R + \Delta r_A), c_\downarrow^\dagger(R + \Delta r_A), c_\uparrow^\dagger(R + \Delta r_B), c_\downarrow^\dagger(R + \Delta r_B))$ is the creation operator of electrons, while $\Delta r_A = -1/4$ and $\Delta r_B = 1/4$ specify the position of sublattices A and B within a unit cell (Fig. 3.1). The matrix σ_- is unity for the (B, A) component while vanishes otherwise.

We consider the case of half-filling, i.e. $2N$ electrons. The Hamiltonian has the symmetry $\sigma_z s_z$, and therefore, the space of occupied electron states is equivalent with the eigenspace of $\sigma_z s_z = +1$ when $h > 0$ is sufficiently large and $\hat{H}$ is in an insulating state. Thus, we can concentrate on the projection of $\hat{H}$ onto $\sigma_z s_z = +1$ eigenspace in order to obtain GWFs. When we write $\mathbf{d}_R^\dagger = (c_\uparrow^\dagger(R + \Delta r_A), c_\downarrow^\dagger(R + \Delta r_B))$, the effective Hamiltonian is given by

$$\hat{H}_+ = \sum_{R=0}^{N-1} \mathbf{d}_R^\dagger (-h - \xi \alpha \tau_y) \mathbf{d}_R + \left(\sum_{R=0}^{N-2} \mathbf{d}_R^\dagger i \alpha \tau_- \mathbf{d}_{R+1} + h.c. \right), \quad (3.5.3)$$

and occupied states of $\hat{H}$ are given by all the eigenstates of $\hat{H}_+$. Corresponding Hamiltonian with periodic boundary condition is given by

$$\hat{H}_+^{\text{PBC}} = \sum_k \mathbf{d}_k^\dagger (-h - \xi \alpha \tau_y + i \alpha \tau_- e^{ik} - i \alpha \tau_+ e^{-ik}) \mathbf{d}_k \quad (3.5.4)$$

$$= \sum_k \mathbf{d}_k^\dagger (-h + \alpha (\cos k - \xi) \tau_y - \alpha \sin k \tau_x) \mathbf{d}_k. \quad (3.5.5)$$

This is essentially the Su-Schrieffer-Herger model with the pseudo spin τ_μ , and is topologically nontrivial for $|\xi| < 1$.

For simplicity of the analysis, we consider the topological limit $\xi = 0$. The situation is schematically shown in Fig. 3.1. The Hamiltonian $\hat{H}_+$ is diagonalized by the intercellular bonding and antibonding orbitals as shown in the panel (a) of Fig. 3.1, for the case of $N = 5$. Therein we showed a possible choice of GWFs, which satisfy the required conditions

1. Spatially localized,
2. Coincide with the genuine (multiband) Wannier functions⁴ in PBC when R is away from the surface,
3. Span the space of occupied electron states in open boundary condition.

In this case, we clearly have a finite spin expectation value around the surface, leading to finite contribution of $\sum_{R,\mu} R \langle W_\mu(R) | \hat{s}_z | W_\mu(R) \rangle$ to spin density polarization. The other basis choice of GWFs is also possible. Examples include the panel (b) and (c) of Fig. 3.1. In the panel (b), we slightly mix the bonding and antibonding orbitals of the panel (a), to carry finite spin expectation values whose sign is highlighted with red (positive) and blue (negative). In this case, the total contribution from GWFs associated with the left-end unit cell to $\sum_{R,\mu} R \langle W_\mu(R) | \hat{s}_z | W_\mu(R) \rangle$ changes in a way proportional to the mixing ratio, while the contribution from the bulk still vanish. The panel (c) shows the case where surface spin expectation values vanish. These examples illustrate the dependence of the surface term in spin density polarization on the basis choice of GWFs.

⁴Here, multiband Wannier functions mean that unitary transformation within occupied bands are allowed [156]. Such unitary transformation is generally required to ensure the localization property, when some bands are entangled with each other. The GWFs of panel (b) and (c) for bulk unit cells give examples of the multiband Wannier functions.

3.6 Summary

In this chapter, we proved spectral bulk-boundary correspondence, which has been only illustrated with specific models [14]. The essential points of the proofs are the analogy with electric polarization. Chirality charges satisfy charge neutrality conditions and equation of continuity, which enables us to prove the relation based on Wannier functions and adiabatic deformation of the Hamiltonian, respectively. We also pointed out that SBBC can be regarded as an extension of the theory of electric polarization to antisymmetries. We clarified that gauge-invariance as well as charge neutrality conditions are essential for a well-defined ‘bulk-boundary correspondence’ of polarizations.

Our discussion is limited to chiral symmetric one-dimensional systems, although the results are also applied to higher-dimensional systems by fixing a $\mathbf{k}$ point in the surface Brillouin zone or just by summing up the contribution from all the $\mathbf{k}$ points in the surface Brillouin zone. It is an interesting future question whether SBBC is generalized to, for example, 3D winding number and interacting systems.

Chapter 4

Conclusion

In this thesis, we studied a novel topological superconductivity and bulk-boundary correspondence.

In Chapter 2, we studied $\mathbb{Z}_4$ and $\mathbb{Z}_2$ topological crystalline superconductivity ensured by glide symmetry. We found that the $\mathbb{Z}_4$ and $\mathbb{Z}_2$ invariants are simplified in the presence of coaxial screw symmetry, following the Fu-Kane criteria for the band inversion of topological insulators [106, 107], as well as Fermi-surface formulas for odd-parity superconductors [57, 108]. The formulas are further simplified by assuming the full symmetry of the space group $Pnma$, which enabled us to relate the topological invariants with the number of Fermi surfaces. We showed that the paramagnetic superconducting phase of UCoGe is topologically nontrivial, by applying the formulas to the Fermi surfaces of UCoGe previously obtained by first-principle calculations [9, 10, 11]. It was found that out of four odd-parity representations of D_{2h} , i.e. A_u , B_{1u} , B_{2u} , and B_{3u} , three odd-parity representations A_u , B_{1u} , and B_{3u} are $\mathbb{Z}_4$ nontrivial, while the three representations B_{1u} , B_{2u} , and B_{3u} are $\mathbb{Z}_2$ nontrivial (B_{1u} and B_{3u} are both $\mathbb{Z}_4$ and $\mathbb{Z}_2$ nontrivial). Thus, the paramagnetic superconducting phase of UCoGe is the first promising material candidate of $\mathbb{Z}_4$ topological glide superconductivity, as well as the second material candidate of $\mathbb{Z}_2$ topological glide superconductivity.

In Chapter 3, we studied novel bulk-boundary correspondence named spectral bulk-boundary correspondence (SBBC) [14], which has not been proved before. We have shown that SBBC is analogous to electric polarization, by introducing the chirality charge satisfying charge neutrality conditions as well as the continuity equation for the chirality charge. Thereby, we proved SBBC based on Wannier-function formalism and adiabatic deformation of Hamiltonian. The process of derivation also offered us an insight into the condition for the electric-polarization-like bulk-boundary correspondence. Our results, combined with those in Ref. [14], revealed that the bulk properties impose strong constraints on the surface physics in systems with local antisymmetries. This is particularly important for time-reversal symmetric superconductors.

We have contributed to the deeper understanding of the topological properties in su-

perconductors, through the studies presented in Chapter 2 and Chapter 3. It is also an interesting future issue to further develop the theories presented above, as discussed in each chapter.

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