Wavefunction topology of two-dimensional time-reversal symmetric superconductors

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We discuss the topology of the wavefunctions of two-dimensional time-reversal symmetric superconductors. We consider (a) the planar state, (b) a system with broken up-down reflection symmetry, and (c) a system with general spin-orbit interaction. We show explicitly how the relative sign of the order parameter on the two Fermi surfaces affect this topology, and clarify the meaning of the $Z_2$ classification for these topological states.

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I. INTRODUCTION

Topological states of matter have received much recent attention. Best known examples are the two-dimensional integer quantum Hall states. These states can be characterized by the Chern numbers associated with the electronic wavefunctions. At the boundary of the sample, the non-trivial topological structure of these wavefunctions necessarily implies the existence of chiral edge states. These states can carry charge (Hall) currents even though the bulk is gapped. Chern numbers can be finite in systems only with broken time reversal symmetry, which in this case is provided by the external magnetic field. Recently, there is much interest in time-reversal symmetric topological insulators. These insulators cannot be classified by the Chern numbers, yet they are topologically distinct from ordinary insulators we learnt in standard solid state textbooks. The role of the $Z_2$ topological number in these systems has been elucidated recently, especially by Kane and his collaborators. There are also surface bound states at the edges of a topological insulator. For a two-dimensional topological insulator, there exist a pair of one-dimensional edge states, related by time-reversal symmetry, at the boundary of the system. In the absence of spin-orbit interaction, these edge states can be regarded as two one-dimensionally dispersing states of opposite spins traveling with opposite velocities. These pair of states can carry spin current, even though the bulk states are gapped. These topologically insulating states are often also referred to as spin-Hall insulators.

There are directly analogies of topological states in superconductors. Here, while the system possesses an extra mechanism of transport via motion of Cooper pairs, the quasiparticle wavefunctions can have topological properties imposed upon them by the order parameter similar to those discussed above. Neither is one restricted to a periodic system; the discussion can be done also in the continuum case. A direct analogy to the integer quantum Hall states are spinless weak-coupling superconductors where the order parameter are $(k_x + i k_y)^n$, where $k_{x,y}$ are the components of the wavevector $\vec{k}$ and $n$’s are (odd) integers. For the continuum, there is no limit to the magnitude of $\vec{k}$. The Chern number is $n$. For $n = 1$, we have the familiar two-dimensional $p$ wave superconductor which possesses a chiral gapless state at the edge of the sample. The non-trivial topology of this state is also reflected in the bound state spectra in a singly quantized vortex. In this case, one finds a Majorana mode at exactly zero energy. Majorana vortex bound states and edge modes are intimately related to each other.

The direct analogy of a time-reversal symmetric topological insulator in two-dimensional is the state often referred to as the "planar state" in the $^3$He literature. Physically, this state is a "equal spin pairing state" where the up and down spins pair only among themselves (but not with each other), with the down (up) spins paired into a $(k_x + i k_y)$ ($k_x - i k_y$) state. This state is obviously time-reversal symmetric. Since the up and down spins are decoupled, it is also clear that the boundary of such a two-dimensional system would have one edge state for each spin species, propagating in opposite directions (see also). A singly quantized vortex in the planar state has two Majorana modes, one for each spin species. In contrast, an s-wave superconductor is topologically trivial. It has no topologically required edge states at the sample boundaries. No Majorana mode exists in its vortex core, and the lowest energy bound state has a finite energy.

What is the fate of this superconducting state when the spins are no longer decoupled? Besides basic theoretical curiosity, this question has now an added significance due to the study of non-centrosymmetric superconductors. These systems include three dimensional systems such as $\text{CePt}_3\text{Si}$ and related compounds, or two-dimensional systems at the interface between two different materials. Consider here in particular a two-dimensional system without up-down reflection symmetry, though still with rotation symmetry about the normal to the plane. In this
system, the planar state is indistinguishable from the s-wave pairing state by symmetry, so the two order parameters can coexist\textsuperscript{26}. However, an s-wave state is topologically trivial, so there must be a non-trivial interplay between the two order parameters when they are simultaneously present. In an earlier paper\textsuperscript{27,28}, we investigated the presence or absence of zero energy modes at the vortex core for such a state. There we find that the zero energy modes exist only if the p-wave order parameter is larger than the s-wave order parameter at the Fermi surface. In addition, we have included a Rashba energy term in the single particle Hamiltonian, which spin-splits the Fermi surface into two according to helicity. We concluded in this case that the existence or absence of the zero energy states is determined by the relative sign of the pairing order parameter on these two Fermi surfaces\textsuperscript{27}

The edge states at the boundary of a two dimensional non-centrosymmetric superconductor have also been studied in\textsuperscript{28}. There the authors have found the conditions on existence or absence of edge states consistent with what we have stated above. (see also\textsuperscript{29} for further discussions)

In this paper, motivated by the above, we try to understand the results of ref\textsuperscript{27,28} by directly examining the topology of the quasiparticle wavefunctions in the bulk. A fundamental concept in topological states is ”obstruction”, that is, the inability to construct a wavefunction smooth in some parameter space (here momentum space) satisfying certain of the quasiparticle wavefunctions in the bulk. A fundamental concept in topological states is “obstruction”, that is, the inability to construct a wavefunction smooth in some parameter space (here momentum space) satisfying certain basic criteria. For the integer quantum Hall state, this has been illustrated explicitly by Kohmoto\textsuperscript{30}. There he showed that, for electrons in a lattice and in the presence of a magnetic field (with rational flux quanta per unit cell), one cannot have a Bloch wavefunction that is smoothly defined throughout the entire (magnetic) Brillouin zone. Dividing the momentum space into two regions, he then showed that the transformation function relating these two regions (also known as the ”transition function”) reflects the finite Chern number of the state. Similar consideration has been utilized by Fu and Kane (Appendix A of\textsuperscript{30}): an insulator is topologically non-trivial if one cannot construct a pseudospin basis smooth within the Brillouin zone (more precise statements below). A transformation function is then used to define the $Z_2$ topological number. We shall follow the same route here for our superconducting states, with $\vec{k}$ however which can extend to infinity. We shall see directly how the relative sign of the order parameter on the Fermi surfaces determines whether it is possible or not for the wavefunction to be smooth in $\vec{k}$ space. This thus in turn determines the $Z_2$ topological classification of the superconducting state.

While preparing the present manuscript, a preprint\textsuperscript{31} on the topology of time-reversal symmetric weak-pairing superconductors in general dimensions appears, employing a method that is very different from ours. These authors started from the quasiparticle Hamiltonian rather than the wavefunctions. For three-dimensions, they developed their classification by employing a topological invariant introduced earlier\textsuperscript{10}. Their classification in two-dimensions is then obtained by performing a dimensional reduction from three-dimensions. For multi-Fermi surfaces, they showed that the product of the signs of the order parameter on Fermi surfaces enclosing time-reversal invariant points determines which $Z_2$ class the superconductor would belong. For a single pair of Fermi surfaces enclosing $\vec{k} = 0$, their result reduces to what we have stated above. The arguments in Ref\textsuperscript{31}, though general, are in a rather abstract form. For two-dimensions, they also rely on an artificial extension of the physical system to an extra dimension. We hope that some readers would find our explicit consideration here of obstruction and transformation function within the physical system more easily understandable and informative.

Our paper is organized as follows. For clearer explanations, we first start with the pure planar state, then introduce $s$-wave mixing and Rashba interaction. We shall explicitly construct the $Z_2$ invariant. Finally, we generalize to a general two-dimensional time-reversal symmetric state. The Appendix contains some technical details.

II. OBSTRUCTION AND THE TRANSFORMATION MATRIX

A. Planar phase

We begin by considering a superconductor (superfluid) in the planar state. The Hamiltonian is given by

$$H_K = \sum_{\vec{k},\alpha} \left( \frac{k^2}{2m} - \mu \right) a_{\vec{k},\alpha}^\dagger a_{\vec{k},\alpha}$$

(1)

and the pairing term $H_{pair} \rightarrow H_{pair}^{planar}$, with

$$H_{pair}^{planar} = \frac{1}{2} \sum_{\vec{k}} \left( i\Delta_p(k) e^{-i\phi_k} a_{\vec{k},1}^\dagger a_{-\vec{k},1}^\dagger + i\Delta_p(k) e^{i\phi_k} a_{\vec{k},1} a_{-\vec{k},1}^\dagger + h.c. \right)$$

(2)
$k$, $\phi_k$ are the magnitudes and azimuthal angles of $\vec{k}$, $\alpha = \uparrow, \downarrow$ the spins, $a_{\vec{k},\alpha}$ is the corresponding annihilation operator, and $h.c.$ denotes the Hermitian conjugate. $m$ is the mass and $\mu$ is the chemical potential. $\Delta_p(k)$, which depends only on the magnitude of $\vec{k}$, is chosen real. In eq (2), the up (down) spins have angular momentum $\mp 1$. To have a Hamiltonian smooth in $\vec{k}$ space, we shall require that $\Delta_p(k) \to 0$ as $k \to 0$. We shall adopt the following convention for the time reversal operator $\Theta$: $\Theta a_{\vec{k},\uparrow}^\dagger \Theta^{-1} = a_{\vec{k},\downarrow}^\dagger$ and correspondingly $\Theta a_{\vec{k},\downarrow} \Theta^{-1} = -a_{\vec{k},\uparrow}$. The Hamiltonian is time reversal invariant, for example $\Theta e^{-i\phi_k} a_{\vec{k},\uparrow}^\dagger a_{\vec{k},\downarrow} a_{\vec{k},\downarrow}^\dagger a_{\vec{k},\uparrow}^\dagger \Theta^{-1} = ie^{i\phi_k} a_{\vec{k},\uparrow}^\dagger a_{\vec{k},\downarrow}^\dagger - a_{\vec{k},\downarrow}^\dagger a_{\vec{k},\uparrow}^\dagger$. In principle we can also choose an $H_{\text{planar}}^\text{pair}$ which is time-reversal invariant under $\Theta$ only after an additional gauge transformation, but this would not add any new physics and we avoid such complications. We could also have chosen a different $H_{\text{planar}}^\text{pair}$ such as $\Delta_p(k)e^{-i\phi_k} a_{\vec{k},\uparrow}^\dagger a_{\vec{k},\downarrow} - \Delta_p(k)e^{i\phi_k} a_{\vec{k},\downarrow}^\dagger a_{\vec{k},\uparrow}$, but this would amount to replacing $\phi_k$ in eq (2) by $\phi_k - \frac{\pi}{2}$ (that is, a relative spin-orbit rotation. This state corresponds to the one used in $20$). Thus eq (2) is the most general planar state. The $i$ factors in this equation are chosen for convenient comparison with the case with finite spin-orbit interactions (subsection B) below.

This Hamiltonian can be easily diagonalized by Bogoliubov transformation, since the two spin species are decoupled. The energies are given by $\pm E(k)$ where $E(k) \equiv \sqrt{\xi^2(k) + \Delta_p^2(k)}$, each doubly degenerate due to spin. Here $\xi(k) = \frac{k^2}{2m} - \mu$. The unoccupied positive energy states $32 |\Psi_1^+(\vec{k})>$, $|\Psi_1^-(\vec{k})>$ have wavefunctions $33$ given by, in the standard notation in spin and particle-hole space,

$$\Psi_1^+(\vec{k}) = N^A \begin{pmatrix} 1 \\ 0 \\ -i\Delta_p(k)e^{i\phi_k}/(E(k) + \xi(k)) \end{pmatrix}$$

$$\Psi_1^-(\vec{k}) = N^A \begin{pmatrix} 0 \\ 1 \\ 0 \\ -i\Delta_p(k)e^{-i\phi_k}/(E(k) + \xi(k)) \end{pmatrix}$$

Here $N^A$ is a normalization constant, which we choose to be real and thus $N^A \equiv ((E(k) + \xi(k))/2E(k))^{1/2}$. For a given $\vec{k}$, $|\Psi_1^+(\vec{k})>$ and $|\Psi_1^-(\vec{k})>$ form a complete set for the positive energy states of the Hamiltonian $H$. In writing eqs (3) and (4) we have required that they satisfy the criteria for a good pseudospin pair as stated in Appendix of $12$ (their eq (A1)), that is,

$$\Theta |\Psi_1(\vec{k})> = |\Psi_2(-\vec{k})>$$

and correspondingly

$$\Theta |\Psi_2(\vec{k})> = -|\Psi_1(-\vec{k})>$$

when $1 \rightarrow \uparrow$ and $2 \rightarrow \downarrow$.

We shall limit ourselves to the case where $\Delta_p(k)$ grows slower than $k^2$ as $k \to \infty$, so that $\Delta_p(k)/(E(k) + \xi(k)) \to 0$ in this limit. Then $|\Psi_1^+(\vec{k})>$ and $|\Psi_1^-(\vec{k})>$ are both well-defined as $\vec{k} \to \infty$. However, these wavefunctions are ill-defined at the origin $\vec{k} \to 0$ if the chemical potential $\mu$ is positive. As $k \to 0$, $\Delta_p(k)/(E(k) + \xi(k)) = (E(k) - \xi(k))/\Delta_p(k) \to \infty$, since $\xi(k) \to -\mu < 0$ and $\Delta_p(k) \to 0$. Hence in this limit $35$

$$\Psi_1^+(\vec{k}) \to (0, 0, -ie^{i\phi_k}, 0)$$

$$\Psi_1^-(\vec{k}) \to (0, 0, -ie^{-i\phi_k})$$

obviously ambiguous at $\vec{k} = 0$.

We can however make the alternative choice,
\[ \Psi^B_\uparrow(\vec{k}) = N^B \begin{pmatrix} i\Delta_p(k)e^{-i\phi_k}/(E(k) - \xi(k)) & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \] (7)

\[ \Psi^B_\downarrow(\vec{k}) = N^B \begin{pmatrix} i\Delta_p(k)e^{i\phi_k}/(E(k) - \xi(k)) & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \] (8)

satisfying the requirements eqs (5) and (6). Here \( N^B \equiv ((E(k) - \xi(k))/2E(k))^{1/2} \). These wavefunctions are well-defined at the origin. As \( k \to 0 \), \( \Delta_p(k)/(E(k) - \xi(k)) \to 0 \), so

\[ \Psi^B_\uparrow(\vec{k}) \to (0, 0, 1, 0) \]

\[ \Psi^B_\downarrow(\vec{k}) \to (0, 0, 0, 1) \]

However, they are ill-defined as \( k \to \infty \). In this limit, \( \Delta_p(k)/(E(k) - \xi(k)) = (E(k) + \xi(k))/\Delta_p(k) \to \infty \) so

\[ \Psi^B_\uparrow(\vec{k}) \to (ie^{-i\phi_k}, 0, 0, 0) \]

\[ \Psi^B_\downarrow(\vec{k}) \to (0, ie^{i\phi_k}, 0, 0) \]

and have values which are \( \phi_k \)-dependent.

Thus \( |\Psi^A_\uparrow(\vec{k})| \) forms a good pseudospin basis for any \( \vec{k} \) excluding the origin, while \( |\Psi^B_\downarrow(\vec{k})| \) is good for any \( \vec{k} \) except at infinity. To have a good pseudospin basis for all \( \vec{k} \), one must divide the \( \vec{k} \) space into two parts, say \( k \geq K \) and \( 0 \leq k \leq K \) for some \( K \), and use respectively \( |\Psi^A_\uparrow(\vec{k})| \) and \( |\Psi^B_\downarrow(\vec{k})| \) in these two regions. For our specific example, \( K \) can assume any finite non-zero value. At the boundary between these two regions (here \( k = K \)), we consider the unitary transformation matrix \( t^{AB} \) between these two basis (see Appendix A of [2], though the details of our analysis is different from this reference; see also [35,36]), with matrix elements defined by

\[ t^{AB}_{ij}(\phi) \equiv |\Psi^A_i(\phi)|\Psi^B_j(\phi) >_{k=K} \] (9)

which is now a function of the angle \( \phi \) (with \( K \) a parameter). The requirements eq (5) (6) impose a non-trivial constraint on this matrix. We have

\[ (|\Psi_1(\phi + \pi)|, |\Psi_2(\phi + \pi)|, \Theta |\Psi_1(\phi)|, |\Theta |\Psi_2(\phi)| >_k = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \] (10)

for both A and B and

\[ t^{AB}(\phi + \pi) = \begin{pmatrix} <\Psi^A_1(\phi + \pi)| & <\Psi^A_2(\phi + \pi)| \\ <\Psi^B_1(\phi + \pi)| & <\Psi^B_2(\phi + \pi)| \end{pmatrix}_k \] (11)

We therefore find

\[ t^{AB}(\phi + \pi) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} t^{AB}(\phi)^* \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \] (12)

Since \( t^{AB} \) is unitary, we can write \( t^{AB} = e^{i\chi(\phi)}G(\phi) \) where \( G(\phi) \) is an element in \( SU(2) \) (\( \det G = 1 \)) [35] and \( G(\phi) \) is required to be smooth. Hence we have

\[ e^{i\chi(\phi + \pi)}G(\phi + \pi) = e^{-i\chi(\phi)}G(\phi) \] (13)

and so there are two possibilities, either

\[ e^{i\chi(\phi + \pi)} = e^{-i\chi(\phi)} G(\phi + \pi) = G(\phi) \] (14)
Fermi surfaces, it is sufficient to consider only pairing terms on the same band and \((\phi + \pi)\). We shall refer \(\Theta_{a} \phi\) that is, if we consider the map from \(\phi \in [0, \pi]\) to \(G(\phi)\), the SU(2) part of \(t^{AB}\), it must be either periodic (eq \((14)\)) or antiperiodic (eq \((15)\)). We note that, if this map is antiperiodic, there is no smooth deformation of the wavefunction which can turn it to be periodic, and so the periodic versus antiperiodic boundary condition can be used for a topological classification \((Z_{2})\). Note also that once \(G(\phi)\) is given between 0 and \(\pi\), its value between \(\pi\) and 2\(\pi\) would then be given.

For our specific example, we can work out easily

\[
t^{AB}(\phi) = \begin{pmatrix}
i e^{-i\phi} & 0 \\
0 & i e^{i\phi}
\end{pmatrix}
\]  

(16)

and so

\[
G(\phi) = \begin{pmatrix}
e^{-i\phi} & 0 \\
0 & e^{i\phi}
\end{pmatrix} = e^{-i\phi \tau_{3}}
\]

(17)

where \(\tau_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\), so \(G(\phi)\) is antiperiodic when \(\phi \to \phi + \pi\). We reproduce the well-known result that our p-wave planar state is \(Z_{2}\) non-trivial.

Our result for \(G(\phi)\) can be easily understood, since the two spin species are decoupled. The factors \(e^\mp i\phi\) in its diagonal elements just reflect the \(\mp 1\) Chern numbers for the two spin species. The same calculation for an s-wave superconductor would show that \(G(\phi)\) is periodic (in fact a constant), hence topologically trivial. This example, though elementary, would be useful to understand the more complicated cases below.

### B. Superconductor with Rashba interaction

We now consider a superconducting system without up-down reflection symmetry. This system has now been studied much theoretically (e.g., \(26,27,28,39,40,41\)). First let us consider the normal state. In addition to the kinetic energy \(H_{K}\) quadratic in \(k\), we now add the Rashba (single-body) term

\[
H_{R} = \sum_{k,\alpha,\beta} -\alpha_{R}(k) a_{k,\alpha}^{\dagger} (\hat{z} \times \hat{k}) \cdot \vec{\sigma}_{\alpha,\beta} a_{k,\beta}
\]

(18)

Here \(\vec{\sigma}\) are the Pauli spin matrices, and \(\alpha_{R}(k) > 0\) is a measure of the strength of this Rashba "interaction". This term can be regarded as a \(\vec{k}\) dependent magnetic field, pointing along \(\hat{z} \times \hat{k}\), thus the system is still rotationally symmetric about its normal. We shall take \(\alpha_{R}(k) \to 0\) as \(k \to 0\), so that \(H_{R}\) is well-defined there. In the normal state, the eigen-energies can easily be seen to be \(\xi_{\pm}(k) = \pm \alpha_{R}(k) - \mu\), according to whether the spin is parallel or anti-parallel to the effective field at \(\vec{k}\), and we shall denote these two bands as \(\pm\). These two bands thus have different Fermi radii \(k_{F,\pm}\). The spin dependent part of the wavefunctions can be chosen as

\[
|\vec{k}^{+}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\
i e^{i\phi_{\vec{k}}}
\end{pmatrix}
\]

(19)

\[
|\vec{k}^{-}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i e^{-i\phi_{\vec{k}}} \\
1
\end{pmatrix}
\]

We note that \(\Theta|\vec{k}^{+}\rangle = ie^{-i\phi_{\vec{k}}} |\vec{k}^{+}\rangle = \Theta|\vec{k}^{-}\rangle = -ie^{i\phi_{\vec{k}}} |\vec{k}^{-}\rangle\) and thus \(\Theta a_{k,\alpha}^{\dagger} a_{k,\beta} = e^{-i\phi_{\vec{k}}} a_{\vec{k}^{+},\alpha}^{\dagger} a_{\vec{k}^{-},\beta}\). We note that \(|\vec{k}^{\pm}\rangle\) do not form a good pseudospin basis since they do not satisfy eq \((4)\) and \((9)\). We shall refer \(\pm\) as helicity indices.

For the superconducting state, in the limit where the pairing is weak compared with the splitting between the two Fermi surfaces, it is sufficient to consider only pairing terms on the same band\(^{40}\). Thus we can write

\[
H_{\text{pair}} = \frac{1}{2} \sum_{\vec{k}} \left( i \Delta_{+}(k) e^{-i\phi_{\vec{k}}} a_{\vec{k}^{+},\alpha}^{\dagger} a_{\vec{k}^{-},\alpha}^{\dagger} - i \Delta_{-}(k) e^{i\phi_{\vec{k}}} a_{\vec{k}^{-},\alpha}^{\dagger} a_{\vec{k}^{+},\alpha}^{\dagger} + \text{c.c.} \right)
\]

(20)
$H_{\text{pair}}$ is time reversal invariant if both $\Delta_{\pm}(k)$ are real, since we have, e.g., $\Theta ie^{-i\phi}\epsilon a^\dagger_{\vec{k}+,\alpha} a^\dagger_{\vec{k}+,\beta} \Theta^{-1} = ie^{-i\phi}\epsilon a^\dagger_{\vec{k}+,\alpha} a^\dagger_{\vec{k}+,\beta}$. The origin of the $e^{-i\phi}$ terms here should not be confused with those in eq (23); they are the result of the choice eq (19) and do not necessarily imply p-wave pairing\textsuperscript{26,41}. Using eq (19) we can rewrite $H_{\text{pair}}$ in terms of ordinary spins and find

$$H_{\text{pair}} = \frac{1}{2} \sum_{\vec{k},\alpha,\beta} \left( a^\dagger_{\vec{k},\alpha} \Delta_{\alpha\beta} a_{\vec{k},\beta} + \text{c.c.} \right)$$

(21)

with

$$\Delta(\vec{k}) = \left( \begin{array}{cc} \frac{\Delta_+(k) + \Delta_-(k)}{2} e^{-i\phi_k} & \frac{\Delta_+(k) - \Delta_-(k)}{2} e^{i\phi_k} \\ \frac{\Delta_+(k) - \Delta_-(k)}{2} e^{-i\phi_k} & \frac{\Delta_+(k) + \Delta_-(k)}{2} e^{i\phi_k} \end{array} \right)$$

(22)

Thus it is a linear combination of s and p-wave planar pairing, with $\Delta_s(k) = \frac{\Delta_+(k) + \Delta_-(k)}{2}$ and $\Delta_p(k) = \frac{\Delta_+(k) - \Delta_-(k)}{2}$. If $\Delta_+(k) = \Delta_-(k)$ for all $k$, we have pure s-wave pairing, and if $\Delta_+(k) = -\Delta_-(k)$, $H_{\text{pair}}$ reduces to $H_{\text{planar}}$. Generally $\Delta_+(k) = \Delta_+(k) \pm \Delta_-(k)$. For ease of discussions below, we shall always assume that $\Delta_+(k)$ is positive, where as $\Delta_-(k)$ may change sign as a function of $k$.

As $k \to \infty$, all pairing terms are negligible compared with the kinetic energy $k^2/2m$, and so the system is effectively normal. To avoid the complications as mentioned below eq (19) we shall require further that $\alpha_R(k) \to 0$ there so that we can easily write down a good pseudospin pair

$$\Psi^D_1 = (1,0,0,0)$$

$$\Psi^D_2 = (0,1,0,0)$$

(23)

which is in fact the same as $|\Psi^A>$ defined in the last subsection in this $k \to \infty$ limit. At $k \to 0$, since $\Delta_p$ vanishes, the pairing either vanishes completely, or is always s-wave like only. Since $\alpha_R(k)$ there vanishes as well, we can have a pair of good pseudospin wavefunctions, which we write as

$$\Psi^D_1 = N^{D2} \begin{pmatrix} 0 \\ -\Delta_s(0)/(E(0) - \xi(0)) \\ 1 \\ 0 \end{pmatrix}$$

$$\Psi^D_2 = N^{D2} \begin{pmatrix} \Delta_s(0)/(E(0) - \xi(0)) \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

(24)

with $N^{D2} \equiv (\langle E(0) - \xi(0)/2E(0)\rangle)^{1/2}$. Here $\xi(0) = \xi_+(0) = -\mu$ is the kinetic energy as $k \to 0$, and $E(0) \equiv \sqrt{\xi^2(0) + \Delta_0^2}$. For general $\vec{k}$, the Hamiltonian can be easily diagonalized in the $\pm$ helicity basis. The energies are $\pm E_\pm(k)$ with $E_\pm(k) = \sqrt{\xi_\pm^2(k) + \Delta_\pm^2(k)}$. The wavefunctions in ordinary spin and particle hole space can then be found by the transformation eq (19). We can choose

$$\Psi^C_+(\vec{k}) = \frac{N^C}{\sqrt{2}} \begin{pmatrix} 1 \\ i e^{-i\phi_k} \Delta_+(k)/(E_+(k) + \xi_+(k)) \\ -i e^{i\phi_k} \Delta_+(k)/(E_+(k) + \xi_+(k)) \end{pmatrix}$$

(25)

and

$$\Psi^C_-(\vec{k}) = \frac{N^C}{\sqrt{2}} \begin{pmatrix} i e^{-i\phi_k} \\ -\Delta_-(k)/(E_-(k) + \xi_-(k)) \\ i e^{i\phi_k} \Delta_-(k)/(E_-(k) + \xi_-(k)) \end{pmatrix}$$

(26)
where $N_+^{C2}(k) = ((E_+(k) + \xi_+(k))/2E_+(k))^{1/2}$ are normalization constants. These functions are chosen so that they reduce to the normal state wavefunctions eq (19) when $k \to \infty$. They are well-defined for finite $k (0 < k < \infty)$ if $\Delta_-(k)$ does not change sign anywhere for $k < k_{F-}$. (If $\Delta_-(k)$ changes sign at $k^* < k_{F-}$, since $\Delta_-(k)/(E_-(k) + \xi_-(k)) = (E_-(k) - \xi_-(k))/\Delta_-(k)$ and $\xi_-(k^*) < 0$, $(E_-(k) - \xi_-(k))/\Delta_-(k) \to \pm \infty$ according to whether $k$ approaches $k^*$ from the $\text{sgn}\Delta_-(k) > 0$ or $< 0$ side.). However, there is no harm if $\Delta_-(k)$ changes sign for $k > k_{F-}$.

There is an alternative choice of wavefunctions

$$\Psi_+^{C2}(\vec{k}) = \frac{N_+^{C2}}{\sqrt{2}} \begin{pmatrix} \Delta_+(k)/(E_+(k) - \xi_+(k)) \\ ie^{i\phi_+} \Delta_+(k)/(E_+(k) - \xi_+(k)) \\ -ie^{i\phi_+} \\ 1 \end{pmatrix}$$

and

$$\Psi_-^{C2}(\vec{k}) = \frac{N_-^{C2}}{\sqrt{2}} \begin{pmatrix} ie^{-i\phi_-} \Delta_-(k)/(E_-(k) - \xi_-(k)) \\ \Delta_-(k)/(E_-(k) + \xi_-(k)) \\ -1 \\ ie^{-i\phi_-} \end{pmatrix}$$

where $N_-^{C2}(k) = ((E_-(k) - \xi_-(k))/2E_-(k))^{1/2}$. These wavefunctions are well-defined for $0 < k < \infty$ only if there are no sign changes of $\Delta_-(k)$ for $k > k_{F-}$. (Actually $|\Psi_+^{C1}|$ and $|\Psi_+^{C2}|$ are always identical, since we assumed $\Delta_+(k) > 0$. We just write explicitly $|\Psi_+^{C2}|$ again for symmetric purposes.)

To study the topological classification as in subsection 11A we need to construct good pseudospin bases satisfying eq (5) and (6) for different parts of $\vec{k}$ space, and then try to match them at the boundaries. However, $|\Psi_\pm^{C1, C2}|$ do not form good pseudospin bases. The problem is that, as in the normal state, the time reversed partner of the $+$ band is the $+$ band itself. Therefore to have a good pseudospin basis one must have $|\Psi_1(\vec{k})| > \text{proportional to } |\Psi_+^+(\vec{k})|$ over part of the $\vec{k}$ space whereas it is proportional to $|\Psi_-^-(\vec{k})| > \text{proportional to } |\Psi_+^-(\vec{k})|$ in the other, introducing discontinuities in the wavefunctions. Rather than trying to deal with this rather messy situation, we note that the topological classification must be independent of the specific construction of the pseudospin basis. If one has a smoothly defined wavefunction, such as $|\Psi_\pm^{C1, C2}| > \text{above under suitable circumstances, then we should be able to decide the } Z_2 \text{ invariant from these wavefunctions alone.}$ We propose that this can done by studying the SU(2) part of the matrix

$$T(\phi) \equiv < \Psi_+^{D1}(\phi)|\Psi_+^{C}(\phi)>_{k \to \infty} < \Psi_+^{C}(\phi)|\Psi_+^{D2}(\phi)>_{k \to 0}$$

with the matrix elements of each matrix defined as in eq (29). Here $1 \to +$, $2 \to -$ for $|\Psi_\pm^{C}|$, and $C \to C1$ or $C2$ should be chosen so that it is smooth for $0 < k < \infty$. Intuitively, we are trying to consider the transformation between the good pseudospin bases $|\Psi_+^{D1}|$ at $k \to \infty$ and $|\Psi_+^{D2}|$ at $k \to 0$ through intermediate states $|\Psi_+^{C}|$ which are smoothly defined for $0 < k < \infty$. Eq (29) is a special case of a more general formula (3A1) which we shall explain in the Appendix.

We now evaluate eq (29). Let us first consider the case where $\Delta_-(k)$ never changes sign for $k < k_{F-}$, so $|\Psi_\pm^{C1}|$ can be used in eq (29). We obtain

$$< \Psi_+^{D1}|\Psi_+^{C1}>_{k \to \infty} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \text{ie}^{-i\phi} \\ \text{ie}^{i\phi} & 1 \end{pmatrix}$$

independent of the sign of $\Delta_\pm(k)$. For $k \to 0$, we get

$$< \Psi_+^{D2}|\Psi_+^{C1}>_{k \to 0} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\text{ie}^{i\phi} & -\text{sgn}\Delta_-(k_{F-}) \\ 1 & \text{ie}^{-i\phi}\text{sgn}\Delta_-(k_{F-}) \end{pmatrix}$$

Here we have used the fact that $\text{sgn}\Delta_-(k \to 0) = \text{sgn}\Delta_-(k_{F-})$ since $\Delta_-(k)$ never changes sign for $k < k_{F-}$. Thus, for $\text{sgn}\Delta_-(k_{F-}) > 0$, we get

$$T(\phi) = \frac{1}{2} \begin{pmatrix} 1 & \text{ie}^{-i\phi} \\ \text{ie}^{i\phi} & 1 \end{pmatrix} \begin{pmatrix} \text{ie}^{-i\phi} & 1 \\ -1 & -\text{ie}^{i\phi} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

(32)
The presence or absence of zeros of $P$ employ $\mathbf{\hat{k}}$. Since this overlap is evaluated at a given $\mathbf{\hat{k}}$ for $k < k_{F-}$ but not for $k > k_{F-}$, we must employ instead $|\Psi^{C2}_{\pm}>$. We find

$$<\Psi^{D1}|\Psi^{C2}>_{k\rightarrow \infty} = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} 1 & ie^{-i\phi} \sgn \Delta_{-}(k_{F-}) \\ ie^{i\phi} & 1 \end{array} \right)$$

where we have used $\sgn \Delta_{-}(k_{F-})$ = $\sgn \Delta_{-}(k \rightarrow \infty)$. On the other hand,

$$<\Psi^{D2}|\Psi^{C2}>_{k\rightarrow 0} = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} -ie^{i\phi} & -1 \\ 1 & ie^{-i\phi} \end{array} \right)$$

independent of the sign of $\Delta_{-}(k_{F-})$. Hence, if $\sgn \Delta_{-}(k_{F-}) > 0$, we get

$$T(\phi) = \frac{1}{2} \left( \begin{array}{cc} 1 & ie^{-i\phi} \\ ie^{i\phi} & 1 \end{array} \right) \left( \begin{array}{cc} ie^{-i\phi} & 1 \\ -1 & -ie^{i\phi} \end{array} \right) = \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right)$$

as in eq (32), independent of $\phi$. This state is $Z_2$ trivial. If $\sgn \Delta_{-}(k_{F-}) < 0$ instead, we get

$$T(\phi) = \frac{1}{2} \left( \begin{array}{cc} 1 & -ie^{-i\phi} \\ ie^{i\phi} & -1 \end{array} \right) \left( \begin{array}{cc} ie^{-i\phi} & 1 \\ -1 & -ie^{i\phi} \end{array} \right) = \left( \begin{array}{cc} ie^{-i\phi} & 0 \\ 0 & ie^{i\phi} \end{array} \right)$$

as in eq (37). This state is again $Z_2$ non-trivial.

We thus conclude that the system is $Z_2$ trivial or non-trivial according to $\sgn \Delta_{-}(k_{F-}) > (<)0$, correspondingly whether $\Delta_{-}(k) > (<)\Delta_{p}(k)$ at $k_{F-}$, a criterion which we had obtained before by considering the vortex bound states. This result can also be understood from continuity. When changing $\Delta_{-}(k_{F-})$, from say, positive to negative, one must go through the point where $\Delta_{-}(k_{F-}) = 0$, which indicates a gapless phase since then $E_{-}(k_{F-}) = \sqrt{\xi_{-}^2(k_{F-}) + \Delta_{-}^2(k_{F-})}$ would vanish on the Fermi surface $\xi_{-}(k_{F-}) = 0$. Hence if $\Delta_{-}(k_{F-})$ and $\Delta_{-}(k_{F-})$ are of the same sign, then one can smoothly change $\Delta_{+}(k)$ to obtain the s-wave state $\Delta_{+}(k) = \Delta_{-}(k)$ without going through any gapless phase. Similarly, if $\Delta_{-}(k_{F+})$ and $\Delta_{-}(k_{F-})$ are of the opposite sign, then the state is connected to planar state $\Delta_{+}(k) = -\Delta_{-}(k)$.

Fu and Kane also proposed that studying the matrix elements (more precisely, the Pfaffian) of $\Theta$ between wavefunctions at the same $k$ point can distinguish whether the system is $Z_2$ trivial or non-trivial. For the system with only two (un-)occupied states $|\Psi_{1,2}(k)>$, this just amounts to studying the function $P(k) = <\Psi_{2}(k)|\Theta|\Psi_{1}(k)>$. The non-trivial topology of the system is determined by the presence of odd numbers of pairs of point zeros of $P(k)$. Since this overlap is evaluated at a given $k$ (not relating $\pm \hat{k}$) and a transformation of basis would not affect the presence or absence of zeros of $P(k)$, $|\Psi_{1,2}(k)>$ here need not be well-defined pseudospin states in the sense of eq (5) and (6). From our previous calculations, we can also see in our example how $P(k)$ can distinguish $Z_2$ trivial versus non-trivial cases, provided one can use a smooth wavefunction in $k$ for $|\Psi_{1,2}(k)>$. (Here $|\Psi^{C1,C2}_{\pm}(k)>$, except here that zeros of $P(k)$ must now appear as circles. Suppose that $\Delta_{-}(k)$ never changes sign for $k < k_{F-}$, then we can employ $|\Psi^{C1}_{\pm}(k)>$. We find

$$P(k) = <\Psi^{C1}_{\pm}(k')|\Theta|\Psi^{C1}_{\pm}(k)> = N^{-1} C_{1}^{C1} \left[ 1 + \frac{\Delta_{+}(k) \Delta_{-}(k)}{E_{+}(k) + \xi_{+}(k) E_{-}(k) + \xi_{-}(k)} \right]$$

(38)
As \( k \to \infty \), \( P(k) = 1 \), but as \( k \to 0 \), \( P(k) \to \text{sgn} \Delta_+ (0) \text{sgn} \Delta_- (0) = \text{sgn} \Delta_- (0) = \text{sgn} \Delta_- (k_{F -}) \). If \( \Delta_- (k_{F -}) > 0 \), then \( P(0) = 1 \). However, if \( \Delta_- (k_{F -}) < 0 \), then \( P(0) = -1 \), implying \( P(k) \) must vanish at some intermediate \( k \) since \( |\Psi^{C1}_{\pm} (\bar{k})| > \) are smooth. In the special case \( k_{F -} = k_{F -} = k_F \), this zero occurs exactly at \( k_F \), since there \( \xi_+ (k) = \xi_- (k) = 0 \) and so \( P(k_F) = [1 + \text{sgn} \Delta_+ (k_F) \text{sgn} \Delta_- (k_F)]/2 \). If \( k_{F +} \) and \( k_{F -} \) are not equal, it can shown that \( P(k) \) vanishes somewhere between these two Fermi surfaces.

Our calculations above do not apply if \( \Delta_- (k) \) changes sign for both \( k > \) and \( k_{F -} \). If this happens, a further generalization of eq (29) is necessary. We can now write

\[
T(\phi) = <\Psi^{D1}(\phi)|\Psi^{C1}(\phi)>_\infty <\Psi^{C1}(\phi)|\Psi^{C2}(\phi)>_{k_{F -}} <\Psi^{C2}(\phi)|\Psi^{D2}(\phi)>_0
\]  

(39)

This equation is a special case of eq (A13) in the Appendix. Using eq (30), (35) and

\[
<\Psi^{C1}(\phi)|\Psi^{C2}(\phi)>_{k_{F -}} = \begin{pmatrix} 1 & 0 \\ 0 & \text{sgn} \Delta_- (k_{F -}) \end{pmatrix}
\]

(40)

we can easily check that the SU(2) part of \( T \) is periodic or antiperiodic in \( \phi \to \phi + \pi \) depending on whether \( \text{sgn} \Delta_- (k_{F -}) > (\ <) 0 \).

### C. General spin-orbit interaction

We generalize the above to general spin-orbit interaction

\[
H_{so} = \sum_{k, \alpha, \beta} -a_{k, \alpha}^\dagger \vec{h}_k \cdot \vec{\sigma}_{\alpha, \beta} a_{k, \beta}
\]

(41)

We parameterize the direction \( \vec{h}(\bar{k}) \) by the spherical angles \( (\beta_k, \alpha_k) \), and thus we have \( \vec{h}_k = |\vec{h}_k| (\sin \beta_k \cos \alpha_k, \sin \beta_k \sin \alpha_k, \cos \beta_k) \) in Cartesian coordinates. Time reversal invariance requires

\[
|\vec{h}(\phi + \pi, k)| = |\vec{h}(\phi, k)|
\]

\[
\beta(\phi + \pi, k) = \pi - \beta(\phi, k)
\]

\[
\alpha(\phi + \pi, k) = \alpha(\phi, k) + \pi \quad (\text{mod } 2\pi)
\]

(42)

but we shall allow general \( \bar{k} \) dependence for these quantities (cylindrical symmetry would not be enforced). \( |\vec{h}_k| \) will be required to vanish at \( \bar{k} = 0 \), and we shall assume that it is finite for \( 0 < \bar{k} < \infty \) so that the bands are non-degenerate. To have well-defined \( \alpha_k, \beta_k \) cannot be equal to \( 0 \) or \( \pi \). We shall assume that \( \vec{h}_k \) does not cover the entire sphere, so with suitable rotations of the spin quantization axes, this condition can be fulfilled. Otherwise some extra care has to be exercised when using the formulas below, but we shall not go into these complications here. If \( |\vec{h}_k| \) is independent of directions, and further \( \beta_k = \pi/2, \alpha_k = \phi_k + \pi/2 \), then (11) reduces to the Rashba interaction (18).

For the normal state, the eigenfunctions, with energies \( \xi_{\pm}(\bar{k}) = \frac{\bar{k}^2}{2m} \mp |\vec{h}_k| - \mu \), can be chosen to be

\[
|\vec{k}^+ > = \begin{pmatrix} \cos(\beta_k/2) \\ \sin(\beta_k/2) e^{i\alpha_k} \end{pmatrix}
\]

\[
|\vec{k}^- > = \begin{pmatrix} -\sin(\beta_k/2) e^{-i\alpha_k} \\ \cos(\beta_k/2) \end{pmatrix}
\]

generalizing eq (19). We now have the time-reversal relations \( \Theta |\vec{k}^+ > = -e^{-i\alpha_k}|\vec{k}^- > \) and \( \Theta |\vec{k}^+ > = -e^{i\alpha_k}|\vec{k}^- > \). The angular dependent Fermi surfaces will be denoted as \( k_{F +}(\phi) \).

In weak pairing limit so that the pairing is only between degenerate bands, we have

\[
H_{pair} = \frac{1}{2} \sum_{\bar{k}} \left(-\Delta_+ (\bar{k}) e^{-i\alpha_k} a_{k+}^\dagger a_{\bar{k}+} - \Delta_- (\bar{k}) e^{i\alpha_k} a_{k-}^\dagger a_{\bar{k}-} + \text{c.c.}\right)
\]

(44)
generalizing eq \(20\). Here \(\Delta_+ (\vec{k})\) are real. As before, the \(e^{\mp i\alpha g}\) phase factors are due to the wavefunctions \(|\vec{k}^\pm\rangle\). \(H_{\text{pair}}\) obeys time-reversal invariance. It is a mixture of singlet and triplet pairs, but the later is not necessarily a simple planar state. We shall take \(\Delta_+ (\vec{k}) > 0\) always, but \(\Delta_- (\vec{k})\) can take either sign. If the system is to remain gapped, then \(\Delta_-(k_{F-} (\phi))\) must be either all positive or all negative for all angles \(\phi\), a situation which we shall assume. Note that as \(\vec{k} \to 0\), all components of the p-wave pairing must go to zero, with only the s-wave component \(\Delta_s\) surviving. There, \(\Delta_+(0) = \Delta_-(0) = \Delta_s(0)\).

In the limit \(\vec{k} \to \infty (0)\), we again have the good pseudospin basis \(|\Psi^{D1}\rangle > (|\Psi^{D2}\rangle >)\) as in eq \(24\) (eq \(21\)). For \(0 < k < \infty\) we can solve the Hamiltonian again first in the \(\pm\) helicity basis, then perform the transformation using \(43\). These wavefunctions can be written as

\[
\Psi^C_+ (\vec{k}) = N^C_+ \begin{pmatrix}
\cos (\beta g/2) \\
\sin (\beta g/2) e^{i\alpha g} \\
-\sin (\beta g/2) e^{i\alpha g} \Delta_+ (\vec{k}) / (E_+ (\vec{k}) + \xi_+ (\vec{k})) \\
\cos (\beta g/2) \Delta_+ (\vec{k}) / (E_+ (\vec{k}) + \xi_+ (\vec{k}))
\end{pmatrix}
\]

and

\[
\Psi^C_- (\vec{k}) = N^C_- \begin{pmatrix}
-\sin (\beta g/2) e^{-i\alpha g} \\
\cos (\beta g/2) \\
-\cos (\beta g/2) \Delta_- (\vec{k}) / (E_- (\vec{k}) + \xi_- (\vec{k})) \\
-\sin (\beta g/2) e^{-i\alpha g} \Delta_- (\vec{k}) / (E_- (\vec{k}) + \xi_- (\vec{k}))
\end{pmatrix}
\]

These wavefunctions are smooth in \(\vec{k}\) if \(\Delta_- (\vec{k})\) do not change sign for \(\vec{k}\) inside the \(k_{F-}\) Fermi surface (\(\mu > 0\)).

The alternative choice of wavefunctions

\[
\Psi^{C2}_+ (\vec{k}) = N^{C2}_+ \begin{pmatrix}
\cos (\beta g/2) \Delta_+ (\vec{k}) / (E_+ (\vec{k}) - \xi_+ (\vec{k})) \\
\sin (\beta g/2) e^{i\alpha g} \Delta_+ (\vec{k}) / (E_+ (\vec{k}) - \xi_+ (\vec{k})) \\
-\sin (\beta g/2) e^{i\alpha g} \\
\cos (\beta g/2)
\end{pmatrix}
\]

and

\[
\Psi^{C2}_- (\vec{k}) = N^{C2}_- \begin{pmatrix}
-\sin (\beta g/2) e^{-i\alpha g} \Delta_- (\vec{k}) / (E_- (\vec{k}) - \xi_- (\vec{k})) \\
\cos (\beta g/2) \Delta_- (\vec{k}) / (E_- (\vec{k}) - \xi_- (\vec{k})) \\
-\cos (\beta g/2) \\
-\sin (\beta g/2) e^{-i\alpha g}
\end{pmatrix}
\]

are smooth if \(\Delta_- (\vec{k})\) does not change signs for \(\vec{k}\) outside the \(k_{F-}\) Fermi surface.

To study the topology, we consider the matrix

\[
T (\phi) \equiv < \Psi^{D1} (\phi) | \Psi^{C} (\phi) >_{k \to \infty} e^{-i\Delta_0 (\phi) s/2} < \Psi^{C} (\phi) | \Psi^{D2} (\phi) >_{k \to 0}
\]

again as the transformation between \(|\Psi^{D1}\rangle >\) and \(|\Psi^{D2}\rangle >\) via smooth wavefunctions \((C \to C1\) or \(C2\) defined in the intermediate \(\vec{k}\) region. The factor \(e^{-i\Delta_0 (\phi) s/2}\) is to take care of the variation of the wavefunction \(|\Psi^{C} (\phi)\rangle >\) from \(k \to 0\) to \(k \to \infty\), here \(\Delta_0 (\phi) \equiv \alpha (\phi, \infty) - \alpha (\phi, 0)\). For the justification of this formula, see the Appendix.

Going through algebra similar to the last subsection, we find, if \(\Delta_- (k_{F-} (\phi)) > 0\),

\[
T (\phi) = \begin{pmatrix}
\sin (\beta g / 2) e^{-i(\alpha + \alpha_0) / 2} \\
-\cos (\beta g / 2) e^{i(\alpha - \alpha_0) / 2} \\
\cos (\beta g / 2) e^{-i(\alpha + \alpha_0) / 2} \\
\sin (\beta g / 2) e^{i(\alpha - \alpha_0) / 2}
\end{pmatrix}
\]

(50)

Here \(\beta_0 \equiv \beta (0, \infty)\) etc, and we have suppressed the \(\phi\) labels in eq \(50\) to shorten notations. For the Rashba spin-orbit interaction, eq \(51\) reduces to \(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\) we have met before. For here, we note that \(\det T = 1\), so that the \(SU(2)\) part of \(T\) can be simply taken as \(T\) itself. Generally, with eq \(12\), we see that \(T (\phi)\) is periodic when \(\phi \to \phi + \pi\), as \(\Delta_0 (\phi + \pi) = \Delta_0 (\phi)\) (see Appendix), and both \(\sin (\beta g / 2)\) and \(e^{\pm i(\alpha + \alpha_0) / 2}\) change sign. This state is therefore topologically trivial.

If \(\Delta_- (k_{F-} (\phi)) < 0\), we find instead
\[ T(\phi) = \begin{pmatrix} \sin(\beta_\alpha + \beta_0) e^{-i(\alpha_\alpha + \alpha_0)/2} & \cos(\beta_\alpha + \beta_0) e^{-i\Delta_\alpha/2} \\ \cos(\beta_\alpha + \beta_0) e^{i\Delta_\alpha/2} & \sin(\beta_\alpha + \beta_0) e^{i(\alpha_\alpha + \alpha_0)/2} \end{pmatrix} \]  \tag{51}

If \( \beta_\alpha = \pi/2 \) and \( \alpha_\alpha = \phi + \pi/2 \), then this formula reduces to \( ie^{-i\phi_{2\pi}} \) we have met before. Generally, we note now that \( \det T(\phi) = -1 \) independent of \( \phi \), so we can take for example \( G(\phi) = -iT(\phi) \). Using eq (12), we find that \( T(\phi) \), hence \( G(\phi) \), is antiperiodic when \( \phi \to \phi + \pi \), as \( \cos(\beta_\alpha + \beta_0) \) and \( e^{i(\alpha_\alpha + \alpha_0)/2} \) both change sign, showing that again the state is topologically non-trivial.

Let us also examine \( P(\vec{k}) \equiv \langle \Psi^{-C}_{-}(\vec{k})|\Theta|\Psi^{C}_{+}(\vec{k}) \rangle \) with \( C \to C1 \) or \( C2 \). Again \( |P(\vec{k})| = 1 \) at \( \vec{k} = 0 \) or \( \infty \). If \( \Delta_{-}(\vec{k}_{F-}) < 0 \) for all \( \phi \), we can show that again \( P(\vec{k}) \) must vanish somewhere in \( \vec{k} \) space. Explicit calculations show that \( P(\vec{k}) \) is real, so it still must vanish on a line in \( \vec{k} \) space. For \( k_{F+}(\phi) = k_{F-}(\phi) \equiv k_{F}(\phi) \), this happens exactly on the Fermi surface (which in general is not a circle).

### III. CONCLUSION

To conclude, we have considered the topology of two-dimensional time-reversal symmetric gapped superconductors by directly analyzing the quasiparticle wavefunctions, specifically the transformation function between wavefunctions defined in different \( \vec{k} \) space regions. This transformation function allows us to classify these superconductors into two types. For weak-coupling superconductors, we verified that the relative sign of the order parameter on the Fermi surfaces is the crucial parameter which determines the topology, providing a deeper understanding of earlier results on vortex bound states and edge states in these systems.

### IV. ACKNOWLEDGEMENT

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### APPENDIX A

Here we explain the formulas eq (29), (39) used in text. Suppose that we have a well-defined pseudospin basis \( |\Psi^{D1}_{+}(\vec{k})\rangle > \) for \( k \geq k_1 \), and another \( |\Psi^{D2}_{+}(\vec{k})\rangle > \) for \( k \geq 0 \), here \( k_1 \geq k_2 \). Suppose further that we have a solution (but not necessarily satisfying eq (1) and (2)) \( |\Psi^{C}_{+}(\vec{k})\rangle > \) to the Hamiltonian for \( k_1 \geq k \geq k_2 \). Then we consider the matrix

\[ T(\phi, k_1, k_2) \equiv \langle \Psi^{D1}_{+}(\phi)|\Psi^{C}_{+}(\phi)\rangle >_{k_1} e^{-i\Delta_\alpha(\phi)\tau_3/2} \langle \Psi^{C}_{+}(\phi)|\Psi^{D2}_{+}(\phi)\rangle >_{k_2} \]  \tag{A1}

Here \( \Delta_\alpha \equiv \alpha(\phi, k_1) - \alpha(\phi, k_2) \), where \( \alpha(\phi, k) \) was defined in section II.C. The matrix \( T \) is in the same spirit as eq (9) except that we now examine the transformation between the two pseudospin bases \( |\Psi^{D1}_{+}\rangle > \) and \( |\Psi^{D2}_{+}\rangle > \) via an intermediate \( |\Psi^{C}_{+}\rangle > \). The factor \( e^{-i\Delta_\alpha(\phi)\tau_3/2} \) is to compensate for possible variations in \( \alpha_\alpha \) between \( k = k_1 \) and \( k = k_2 \). In this formula, we have limited ourselves to the case where \( \beta_\alpha \) never equals to 0 or \( \pi \). This guarantees that the factor \( e^{-i\Delta_\alpha(\phi)\tau_3/2} \) is well-defined despite that \( \alpha \) is defined only up to mod \( 2\pi \): For a given \( k \), if say \( \alpha(\phi, k) \) increases by \( \pi \) when \( \phi \) advances by \( \pi \), then the same thing must happen for a neighboring \( k' \) since \( \alpha(\phi, k) \) is smooth (instead of, e.g., \( \alpha(\phi, k') \) decreasing by \( \pi \)). Continuing this argument shows that \( \alpha(\phi + \pi, k_1) - \alpha(\phi, k_1) = \alpha(\phi + \pi, k_2) - \alpha(\phi, k_2) \), so that \( \Delta_\alpha(\phi + \pi) = \Delta_\alpha(\phi) \) and \( \Delta_\alpha(\phi + 2\pi) = \Delta_\alpha(\phi) \) without any \( 2\pi \) ambiguities. The precise form of this factor is dependent on the behavior of the helicity basis \( |\Psi^{C}_{+}\rangle \) under time reversal (see eq (A5) below). A more complicated form is necessary for example if we choose to multiply eq (13)-(18) by \( k \) dependent phase factors, which we choose not to do here.

For simplicity, we have also written eq (A11) on two circles \( k_1 \) and \( k_2 \) in \( \vec{k} \) space. Since the system may not be cylindrically symmetric, one can also choose to write this equation on more general paths in \( \vec{k} \) space enclosing the origin, but this would complicate the notation. In the text we have only used this formula for \( k_1 \to \infty \) and \( k_2 \to 0 \).
where \( \det \mathbf{G}^{D1,C} = 1 \) etc. We thus have

\[
T(\phi) = e^{i(\chi^{D1,C}(\phi)+\chi^{C,D2}(\phi))} \mathbf{G}^{D1,C}(\phi)e^{-i\Delta \alpha(\phi)\tau_3/2} \mathbf{G}^{C,D2}(\phi)
\]

\[= e^{ix(\phi)} \mathbf{G}(\phi) \quad (A3)\]

Let us now investigate the consequence of time-reversal symmetry. Eq (12) and (13) require

\[
(|\Psi^{D1}_1(\phi+\pi)>,|\Psi^{D1}_2(\phi+\pi)>)_k = (|\Theta \Psi^{D1}_1(\phi)>,|\Theta \Psi^{D1}_2(\phi)>)_k \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right)
\]

\[= (|\Theta \Psi^{D1}_1(\phi)>,|\Theta \Psi^{D1}_2(\phi)>)_k \left( \begin{array}{cc} -e^{i\alpha(\phi,k)} & 0 \\ 0 & -e^{-i\alpha(\phi,k)} \end{array} \right) \quad (A4)\]

For our helicity basis, we have, from eq (45)-(48)

\[
\left( |\Psi^{C}_+(\phi+\pi)>,|\Psi^{C}_-(\phi+\pi)> \right)_k = \left( |\Theta \Psi^{C}_+(\phi)>,|\Theta \Psi^{C}_-(\phi)> \right)_k \left( \begin{array}{cc} -e^{i\alpha(\phi,k)} & 0 \\ 0 & -e^{-i\alpha(\phi,k)} \end{array} \right) \quad (A5)\]

We thus obtain

\[
t^{D1,C}(\phi+\pi) = \left( \begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right) \left( t^{D1,C}(\phi) \right)^* \left( \begin{array}{cc} -e^{i\alpha(\phi,k)} & 0 \\ 0 & -e^{-i\alpha(\phi,k)} \end{array} \right) \quad (A6)\]

Similarly,

\[
t^{C,D2}(\phi+\pi) = \left( \begin{array}{cc} -e^{-i\alpha(\phi,k_2)} & 0 \\ 0 & -e^{i\alpha(\phi,k_2)} \end{array} \right) \left( t^{C,D2}(\phi) \right)^* \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right) \quad (A7)\]

By judicially inserting 1 = \( \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right) \) and using the commutation properties of Pauli matrices, we find

\[
T(\phi+\pi) = e^{-i(\chi^{D1,C}(\phi)+\chi^{C,D2}(\phi))} \mathbf{G}^{D1,C}(\phi)e^{-i\Delta \alpha(\phi)\tau_3/2} \mathbf{G}^{C,D2}(\phi)
\]

\[= e^{ix(\phi+\pi)} \mathbf{G}(\phi+\pi) = e^{-ix(\phi)} \mathbf{G}(\phi) \quad (A9)\]

thus allowing classifications by the behavior of \( \mathbf{G}(\phi) \) under \( \phi \rightarrow \phi + \pi \) as in section II A.

Eq (A1) is directly related to the transformation used in [12], and formula such as eq (9). The analogy to these would be to study

\[
t^{D1,D2}(\phi) = <\Psi^{D1}(\phi)|\Psi^{D2}(\phi)>_K \quad (A10)\]

at some \( K \) where both \( |\Psi^{D1}(k)> \) and \( |\Psi^{D2}(k)> \) are well-defined. If indeed \( |\Psi^{D2}(k)> \) in eq (A1) is defined for \( k \) up to \( k_1 \), then we see that, using that \( |\Psi^{D2}(k)> \) forms a complete set for the positive energy levels,

\[
T(\phi) = <\Psi^{D1}(\phi)|\Psi^{D2}(\phi)>_{k_1} \mathbf{M}(\phi,k_1,k_2) \quad (A11)\]

where

\[
\mathbf{M}(\phi,k_1,k_2) = <\Psi^{D2}(\phi)|\Psi^{C}(\phi)>_{k_1}e^{-i\Delta \alpha(\phi)\tau_3/2}<\Psi^{C}(\phi)|\Psi^{D2}(\phi)>_{k_2} \quad (A12)\]

so amounts evaluating (A10) at \( k_1 \) and post-multiplying by the matrix \( \mathbf{M} \). By the same analysis as from eq (A1) to (A9), we see that the SU(2) part of \( \mathbf{M} \) must be either periodic or antiperiodic when \( \phi \rightarrow \phi + \pi \). However, since the wavefunctions entering \( \mathbf{M} \) are smooth and \( \mathbf{M}(\phi,k_2,k_2) \) is necessarily simply 1, the SU(2) part of \( \mathbf{M}(\phi,k_1,k_2) \) must be periodic when \( \phi \rightarrow \phi + \pi \). Hence the classification is not affected by the post-multiplication by this matrix.

Similarly, one can show that the classification by the SU(2) part of (A1) is independent of the choice of the pseudospin basis \( |\Psi^{D1}> \) or \( |\Psi^{D2}> \), so long as they are smoothly defined in their respected regions in \( \vec{k} \) space. A different choice would just amount to pre- or post-multiplying eq (A1) by a matrix with the SU(2) part of which being periodic in \( \phi \rightarrow \phi + \pi \).

We have assumed that \( \beta_\vec{k} \) is never 0 or \( \pi \) in eq (A1). When this does not apply, the factor \( e^{-i\Delta \alpha(\phi)\tau_3/2} \) there has to be rewritten. The necessary form can be obtained by considering more carefully how eq (A5) changes when \( \vec{k} \) is varied, but we shall not go into these complications here.
When there are sign changes of $\Delta_\pm(k)$ for both outside and inside $k_{F-}$, one must use $|\Psi^{C1}(\phi)\rangle$ and $|\Psi^{C2}(\phi)\rangle$ for these two regions separately. Similar considerations above show that a transformation matrix which can be used is

$$T(\phi, k_1, k_2) \equiv <\Psi^{D1}(\phi)|\Psi^{C1}(\phi)\rangle_{k_1} e^{-i\Delta_1(\phi)\tau_3/2} <\Psi^{C1}(\phi)|\Psi^{C2}(\phi)\rangle_{k_{F-}(\phi)} \times e^{-i\Delta_2(\phi)\tau_3/2} <\Psi^{C2}(\phi)|\Psi^{D2}(\phi)\rangle_{k_2}$$

(A13)

where $\Delta_1(\phi) \equiv \alpha(\phi, k_1) - \alpha(\phi, k_{F-}(\phi))$ and $\Delta_2(\phi) \equiv \alpha(\phi, k_{F-}(\phi)) - \alpha(\phi, k_2)$. If $\alpha$ is independent of $k$, this formula reduces to eq (39) at the end of section II B.

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33. We have removed the plane wave factors $e^{ik_Fr}$ of these wavefunctions before discussing the topology, as also done in e.g. 4,5,6,30. We however would not introduce another symbol for simplicity in notations.
34. The wavefunction of the time reversed state can be obtained by complex conjugation and then pre-multiply by the matrix

$$
\begin{pmatrix}
0 & -1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 \\
0 & 0 & 1 & 0
\end{pmatrix}
$$

(A14)

Note $\phi_{-g} = \phi_g + \pi \bmod 2\pi$.
35. When discussing the topology, we regard $k \rightarrow \infty$ as a single point irrespective of its direction, as done in 16 etc. We shall therefore require well-defined pseudospin wavefunctions to have $\phi$ independent values as $k \rightarrow \infty$. This condition would not be imposed on wavefunctions such as $|\Psi^C\rangle$ in subsections II B and II C that are used as intermediate wavefunctions.
Strictly speaking we need a transpose here, but we shall suppress this to simplify notations.

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$G(\phi)$ is still ambiguous up to a $\pm$ sign. However, this does not cause any concern since we would be studying a smooth map $\phi \rightarrow G(\phi)$.

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$|P(k)|$ must be unity at $\vec{k} = 0$ and $\vec{k} = \infty$. In the language of $\mathcal{L}$, these are time-reversal invariant points and must belong to the "even subspace" of $P(k)$. 