**$\mathbb{Z}_2$ Topologically Obstructed Superconducting Order**

Canon Sun and Yi Li  
*Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland 21218, USA*

(Dated: September 16, 2020)

We propose a class of topological superconductivity where the pairing order is $\mathbb{Z}_2$ topologically obstructed in a time-reversal invariant system in three dimensions. When two Fermi surfaces are related by time-reversal and mirror symmetries, such as those in a $\mathbb{Z}_2$ Dirac semimetal, the inter-Fermi-surface pairing in the weak-coupling regime inherits the band topological obstruction. As a result, the pairing order cannot be well-defined over the entire Fermi surface and forms a time-reversal invariant generalization of $U(1)$ monopole harmonic pairing. A tight-binding model of the $\mathbb{Z}_2$ topologically obstructed superconductor is constructed based on a doped $\mathbb{Z}_2$ Dirac semimetal and exhibits nodal gap function. At an open boundary, the system exhibits a time-reversal pair of topologically protected surface states.

**Introduction.** – Central to understanding the properties of a superconductor is the symmetry of its pairing order, which forms irreducible representations of the symmetry of the system. It is usually characterized by the spherical harmonic functions or their lattice counterparts. Notable examples include conventional s-wave superconductors such as Hg and Nb, unconventional p-wave superfluid $^3$He [1–4], p-wave heavy fermion compounds [5–7], and d-wave high-Tc cuprates [8, 9].

Another notion fundamental to unearthing new phases of matter is the topology of electronic bands. In a seminal work, a two-dimensional (2D) insulating system with broken time-reversal symmetry (TRS) has been discovered to exhibit the quantum anomalous Hall effect characterized by a non-zero Chern number [10]. It arises from the geometry of Bloch wave functions whose phase cannot be well defined over the entire 2D Brillouin zone (BZ) [11]. The notion of topology in electronic bands was then generalized to insulators with TRS in two and three dimensions (3D), which are characterized by a $\mathbb{Z}_2$ invariant [12–21]. Furthermore, topological obstructions in metallic bands and quasiparticle states give rise to the notions of topological Fermi liquids, semimetals and superconductors [4, 22–41].

While topological superconductivity has been generally invoked in discussions of topological Bogoliubov-de Gennes (BdG) quasiparticle states, a recent work introduced the notion of monopole superconductivity [42], which captures an $U(1)$ topological obstruction of the phase of the superconducting order [43]. This leads to nodal superconducting gap functions described by monopole harmonic functions [42] which are topological sections of an $U(1)$ bundle over a sphere [44, 45]. The monopole pairing is fundamentally different from the familiar s-, p- and d-wave pairings based on spherical harmonics and is beyond the ten-fold way classification [46]. It can be realized in certain doped Weyl semimetals or spin-orbit coupled cold atom systems [42, 47–49]. The notion of monopole pairing has also been extended to the particle-hole channel and leads to, for example, monopole density wave orders [50].

In this letter, we explore a non-Abelian topological obstruction in superconducting pairing orders characterized by a $\mathbb{Z}_2$ invariant. When two helical FSs are related by time-reversal (TR) and mirror symmetries with their composed symmetry $\mathcal{T}$ satisfying $\mathcal{T}^2 = -1$, the Bloch states at the FSs are classified by a $\mathbb{Z}_2$ topological index. In the weak-coupling regime, when Cooper pairing occurs between $\mathbb{Z}_2$ non-trivial FSs, the topology of Bloch states near FSs induces an $SO(3)$ topological obstruction in the superconducting order which is characterized by a $\mathbb{Z}_2$ invariant. This obstruction is the inability to enforce the symmetry condition imposed by $\mathcal{T}$ on the pairing order globally without introducing singularities, which can be made regular by relaxing the symmetry condition through the introduction of the sewing matrix. An example of $\mathbb{Z}_2$-obstructed pairing is explored in a tight-binding model of a doped $\mathbb{Z}_2$ Dirac semimetal in proximity to an s-wave superconductor with inter-orbital pairing. The system exhibits a time-reversal pair of topological surface states which form zero-energy Majorana arcs connecting the surface projections of bulk gap nodes.

**Topologically $\mathbb{Z}_2$ Fermi Surfaces.** – We begin with a 3D minimal model of a pair of $\mathbb{Z}_2$ obstructed FSs. Consider two disjoint spherical Fermi surfaces, $\text{FS}_{\pm}$, related by TR and ‘mirror’ symmetries centered about $\pm \mathbf{K}_0 = \pm (0,0,K_0)^T$, as shown in Fig. 1 (a). Let $\hat{\Psi}^{\pm}_{a,b}(\mathbf{q})$ denote the fermion creation operator on $\text{FS}_{\pm}$ for the $a$-th band with wavevector $\mathbf{k} = \pm \mathbf{K}_0 + \mathbf{q}$. Here $a = 1, 2$ labels the degrees of freedom on the FSs. The fermion operators on $\text{FS}_{\pm}$ are related to those on $\text{FS}_{\mp}$ by TRS, $\mathcal{T}$, as $\hat{\Theta} \hat{\Psi}^{\pm}_{a,b}(\mathbf{q}) \hat{\Theta}^{-1} = \sum_b \hat{\Psi}^{\mp}_{\mp,b}(-\mathbf{q}) [i\sigma_y]_{ba}$, where $\theta_\mathbf{q} = \phi_\mathbf{q}$ are the polar and azimuthal angles of $\mathbf{q}$, respectively. If the ‘mirror’ symmetry, $\mathcal{M}_z$, satisfies $\mathcal{M}_z \hat{\Psi}^{\pm}_{a,b}(\theta_\mathbf{q},\phi_\mathbf{q}) \mathcal{M}_z^{-1} = \hat{\Psi}^{\mp}_{a,b}(\pi - \theta_\mathbf{q},\phi_\mathbf{q})$, the combination $\mathcal{T} \equiv \mathcal{M}_z \hat{\Theta}$ leads to a new antiunitary symmetry that relates operators on the same FS at the same $k_z$,

$$\mathcal{T} \hat{\Psi}^{\pm}_{a,b}(\mathbf{q}) \mathcal{T}^{-1} = \sum_b \hat{\Psi}^{\mp}_{\mp,b}(\mathbf{q} + \pi \phi_\mathbf{q}) [i\sigma_y]_{ba},$$

(1)
which implies the transition matrix can be continuously along $S_q$ matrices. When the contractible, blue and non-contractible, red loops, respectively, in SU(2) transition matrices in cases (I) and (II) correspond to $N$ $(b)$ The 2D spherical FS is divided into two gauge patches along the $k_\pm$ and $N \cap S$ (green). (c) From Ref. 20, the two topological classes of SU(2) transition matrices in cases (I) and (II) correspond to the contractible, blue and non-contractible, red loops, respectively, in SU(2) $\cong S^3$. (d) The group SO(3) is topologically $\mathbb{RP}^3$. Under the map $G_\pm(q) \mapsto R_\pm(q)$, the two paths in (c) are mapped to paths of the corresponding color in (d).

satisfying $\hat{T}^2 = -1$. This can be viewed as TRS in 2D.

Based on the analysis of physical TRS in 2D topological insulators in Refs. 19 and 20, the symmetry $\hat{T}$ here classifies the Bloch states near a FS into two topological sectors. To illustrate this, let us first focus on FS$_+$ and divide it into two patches, $N$ and $S$, as shown in Fig. 1 (b). Define the fermion operators $\hat{\Psi}_{\pm, \alpha}(q)$ in $N$ as $\hat{\alpha}_{\pm, \alpha}^\dagger(q)$ and those in $S$ as $\hat{\beta}_{\pm, \alpha}^\dagger(q)$ with their respective Bloch states smoothly defined over each patch. Generally, the operators defined on the two patches are related by an U(2) gauge transformation $M_+(q)$ at the overlap,

$$\hat{\alpha}_{\pm, \alpha}^\dagger(q) = \sum_{b=1}^2 \hat{\beta}_{\pm, \beta}^\dagger(q) M_{+, ba}(q), \quad q \in N \cap S. \quad (2)$$

Here, the transition matrix $M_+(q) = e^{i\omega_+(q)G_+(q)}$ consists of an U(1) phase $e^{i\omega_+(q)}$ and SU(2) matrix $G_+(q)$.

In order for the transition matrix to be compatible with $\hat{T}$-symmetry, it is constrained to one of two possible cases [19, 20]: (I) $G_+(q + \pi \phi_\alpha) = G_+(q)$ and (II) $G_+(q + \pi \phi_\alpha) = -G_+(q)$. $G_+$ maps $q \in N \cap S \cong S^1$ to SU(2) matrices. When $q$ is varied from $(\theta_\alpha, \phi_\alpha)$ to $(\theta_\alpha, \phi_\alpha + \pi)$ along $S^1$, $G_+$ traces out a path in SU(2). As shown in Fig. 1 (c), the path in SU(2) is contractible in case (I) which implies the transition matrix can be continuously deformed to the identity, and hence the Bloch states can be smoothly defined over FS$_+$. On the other hand, in case (II), there does not exist such a deformation as the path must visit the antipodal point. This topological obstruction makes it necessary to define the Bloch states using two gauge patches.

The operators on FS$_-$ are in the same topological class as those on FS$_+$. This follows from TRS, which relates the transition matrix on FS$_-$, $M_-(q)$, with $M_+(q)$ via

$$M_-(q) = e^{-i\omega_+(q)}G_+(q). \quad (3)$$

As the transition matrices $M_{\pm}$ share the same SU(2) part, states on FS$_{\pm}$ fall the same topological class.

It is possible to choose Bloch states that are globally well-defined if the $\hat{T}$ condition is not strictly enforced [20, 51]. Let $\hat{\Psi}_{\pm, \alpha}(q) = \hat{\chi}_{\pm, \alpha}(q)$ denote the creation operator for a state that is regular over the entire FS. The condition imposed by $\hat{T}$-symmetry is relaxed to

$$\hat{T}\hat{\chi}_{\pm, \alpha}(q)\hat{T}^{-1} = \sum_b \chi_{\pm, b}(q + \pi \phi_\alpha)w_{+, ba}(q). \quad (4)$$

Here $w_{+, \alpha}(q) = \langle 0|\hat{\chi}_{\pm, \alpha}(q + \pi \phi_\alpha)|\hat{T}\hat{\chi}_{\pm, \alpha}(q)|0\rangle$ are unitary matrices defined on FS$_\pm$, called sewing matrices. Since they are not independent and satisfy $w_{+, \alpha}(\theta_\alpha, \phi_\alpha) = w_{+, \alpha}(\pi - \theta_\alpha, \phi_\alpha)$ as a result of mirror symmetry, let us focus on $w_{+, \alpha}(q)$. Because $\hat{T}^2 = -1$, the sewing matrix satisfies $w_{+, \alpha}(q) = -w_{+, \alpha}(q + \pi \phi_\alpha)$, which makes it antisymmetric at the $\hat{T}$-invariant momenta, namely the north and south poles $(\theta_\alpha = 0, \pi)$. As an unitary matrix, it can be decomposed as $w_{+, \alpha}(q) = e^{i\xi_{+, \alpha}(q)}\tilde{w}_{+, \alpha}(q)$, where $e^{i\xi_{+, \alpha}(q)} \in U(1)$ and $\tilde{w}_{+, \alpha}(q) \in SU(2)$. At the two poles, $\tilde{w}_{+, \alpha}(\theta_\alpha = 0, \pi) = Pf \tilde{w}_{+, \alpha}(\theta_\alpha = 0, \pi)i\sigma_y$ and the $\mathbb{Z}_2$ invariant of FS$_+$ has been defined using the Fu-Kane formula [52]

$$\delta = Pf \tilde{w}_{+, \alpha}(\theta_\alpha = 0) Pf \tilde{w}_{+, \alpha}(\theta_\alpha = \pi), \quad (5)$$

which takes value +1 (−1) in the non-topological (topological) phase. When inversion symmetry, defined as $\hat{\Pi}\hat{\chi}_{\pm, \alpha}(q)\hat{\Pi}^{-1} = \sum_p \hat{\chi}_{\pm, \alpha}(-q)U_p$, where $U_p$ is unitary, is present, $\delta$ reduces to the product of the eigenvalues of the in-plane inversion operator, defined as $\hat{P} \equiv M_+\hat{\Pi}$, at the two $\hat{T}$-invariant points [14, 52]. The equivalence between the two gauges picture and the Fu-Kane invariant is established in Supplementary Material I.

**Topologically Obstructed Superconducting Order.** – The $\mathbb{Z}_2$ obstructed FSs can induce a topological obstruction in the pairing order. Let us consider inter-FS Cooper pairing between FS$_+$ and FS$_-$, as described by the mean-field pairing Hamiltonian

$$\hat{H}_\Delta = \sum_{q, \alpha, \beta} \hat{\alpha}_{\pm, \alpha}^\dagger(q) \Delta_{a_b}^N(q) \hat{\alpha}_{\pm, \beta}^\dagger(-q) + \text{h.c.}, \quad (6)$$

where $\Delta_{a_b}^N(q) = \sum_{q', c_d} V_{abcd}(q, q') \langle \hat{\alpha}_{-c}(-q')\hat{\alpha}_{+, d}(q') \rangle$ is the superconducting gap function defined in the region $N$ of FS$_+$ and $V_{abcd}(q, q')$ is the inter-FS attractive interaction potential. To obtain the gap function in the
region $S$, we perform the gauge transformation in Eq. (2), leading to the relation $\Delta^S(q) = G_+ (q) \Delta^N(q) G^T_+ (q)$, where we have used Eq. (3). It is convenient to decompose the gap function into singlet and triplet sectors, $\Delta^{N/S}(q) = \left(d^N_0(q) + d^N_0(q) \cdot \sigma \right) i \alpha_y$. In this notation, the gap function transforms under the gauge transformation as

$$d^0_0(q) = d^N_0(q)$$

$$d^S(q) \cdot \sigma = G_+ (q) \left(d^N(q) \cdot \sigma \right) G^T_+(q) = \left(R_+(q)d^N(q) \right) \cdot \sigma,$$  

(8)

where $R_+(q)$ is the rotation matrix in the vector representation associated with $G_+ (q)$. The effect of the gauge transformation is a rotation on the spin-0 and spin-1 sectors of the gap function. $d^N_0$ is unaffected by the gauge transformation as it is rotationally invariant. Therefore, for singlet pairing in the band basis the gap function can be smoothly defined over the FS. On the other hand, $d^N(q)$ is generally not invariant under the rotation, with the only exception being when $d^N(q)$ is parallel to the rotation axis. The map $G_+ (q) \rightarrow R_+(q)$ transforms the two classes of paths in SU(2) space to loops in SO(3). As illustrated in Figs. 1 (c) and (d), a path belonging to case (I) is mapped to a contractible loop whereas one in case (II) is mapped to a non-contractible loop, corresponding to the trivial and non-trivial elements of the fundamental group $\pi_1(\text{SO}(3)) \cong \mathbb{Z}_2$, respectively. Therefore, if the FSs are $\mathbb{Z}_2$ non-trivial, the superconducting order parameter associated with triplet pairing is topologically obstructed and requires the use of two gauge patches.

In the sewing matrix approach, it is possible to select a single gauge patch to describe the gap function, at the expense of the $T$-symmetry condition on the $d$ vectors. In the singular gauge, the symmetry $\hat{T}$ imposes on the gap function the constraint $(i\sigma_y) \left[ \Delta^{N/S}(q) \right]^* (i\sigma_y)^T = \Delta^{N/S}(q + \pi \hat{\phi}_q)$. For singlet pairing, this gives $\left[ d^N_0(q) \right]^* = d^N_0(q + \pi \hat{\phi}_q)$ and for triplet pairing $\left[ d^N_0(q) \right]^* = d^N_0(q + \pi \hat{\phi}_q)$.

To study what the $T$-symmetry condition is in the regular gauge, first perform a transformation from $\hat{\alpha}_\pm$ to $\hat{\chi}_\pm(q)$. The gap function in the non-singular basis reads $\Delta(q) = U_+(q) \Delta_N(q) U^T_+(-q)$, where $[U_+(q)]_{ab} = \langle 0|\hat{\chi}_{\pm,a}(q)\hat{\alpha}_{\pm,b}^{\dagger}(q)|0\rangle$. Using mirror and $\hat{T}$ symmetries, the basis transformation matrices are related by $U^T_+(-q) = (-i\sigma_y) U_+^T(q + \pi \hat{\phi}_q)$, and hence

$$\Delta(q) = (d_0(q) + d(q)) w_+(q + \pi \hat{\phi}_q),$$  

(9)

where $d_0 = d_0^N$, $d(q) = D_+(q) d^N(q)$, and $D_+(q)$ is the SO(3) rotation matrix associated with the SU(2) part of $U_+(q)$. In this new basis, the condition imposed by $\hat{T}$-symmetry is $w_+(q) \Delta^*_N(q) U^T_+(-q) = \Delta(q + \pi \hat{\phi}_q)$. For singlet pairing, this simplifies to the same condition as in the singular gauge and thus there is no obstruction to the $\hat{T}$-symmetry condition. In contrast, for triplet pairing, $w_+(q) (d(q) \cdot \sigma)^T w_+^T(q) = d(q + \pi \hat{\phi}_q) \cdot \sigma$. This cannot be reduced to the ordinary time-reversal condition since $\hat{w}_+(\theta_q = 0) = -\hat{w}_+(\theta_q = \pi)$ for a $\mathbb{Z}_2$ non-trivial FS. Consequently, there is an obstruction to enforce the $\hat{T}$-symmetry condition for triplet pairing, in agreement with the result obtained in the singular gauge.

Apart from TRS, mirror symmetry in the fermion BdG Hamiltonian require the pairing matrix satisfying $\Delta^{N/S}(q) = -[\Delta^{N/S}(q + \pi \hat{\phi}_q)]^T$. This implies the gap function for triplet pairing vanishes at the $\hat{T}$-invariant points. In other words, the resulting BdG quasiparticle spectrum is nodal at the poles.

A Model of the $\mathbb{Z}_2$ Pairing Order. – A simple example of $\mathbb{Z}_2$-obstructed pairing can be constructed by considering interacting-pairing in a $\mathbb{Z}_2$ Dirac semimetal [53]: $H = H_0 + H_\Delta$, where $H_0 = \sum_{\alpha, \beta} c^\dagger_{\alpha k} (h(k) - \mu)_{\alpha, \beta} c_{\beta k}$ is a four-band Hamiltonian of a $\mathbb{Z}_2$ Dirac semi-metal and $H_\Delta = \sum_{\alpha, \beta} c^\dagger_{\alpha k} \Delta_{\alpha \beta} (k) c_{\beta k} + h.c.$ describes the mean-field inter-FS pairing. Here, the chemical potential $\mu > 0$, $\Delta_{\alpha \beta}(k)$ is the gap function, and $\tilde{c}_{\alpha k}$ is the creation operator for an electron with wavevector $k$ and index $\alpha$, which labels the orbital and spin degrees of freedom.

The matrix kernel in $H_0$ is $h(k) = \sum_{j=1}^5 h_j(k) \Gamma_j$, where $h_1(k) = m(2 - \cos k_x - \cos k_y - \cos k_z)$, $h_2(k) = t_1 \sin k_x$, $h_3(k) = t_1 \sin k_y$, $h_4(k) = t_2 \sin k_x$, and $h_5(k) = t_2 \sin k_y$. Here $t_1$, $t_2$, and $m$ are hopping parameters which, for simplicity, satisfy $m = \sqrt{2} t_1 = \sqrt{2} t_2$. The gamma matrices $\Gamma_i$ satisfying the Clifford algebra $(\Gamma_i, \Gamma_j) = 2\delta_{ij} \sigma_0 \otimes \tau_0$ are chosen to be $\Gamma_1 = \sigma_0 \otimes \tau_z$, $\Gamma_2 = \sigma_x \otimes \tau_x$, $\Gamma_3 = \sigma_y \otimes \tau_y$, $\Gamma_4 = \sigma_x \otimes \tau_z$, and $\Gamma_5 = \sigma_y \otimes \tau_z$, where $\sigma_0 (\tau_0)$ is the two-by-two identity matrix and $\sigma_1 (\tau_1)$ are the Pauli matrices in spin (orbital) space. There are two Dirac nodes at $\pm K_0 = \pm (0, 0, K_0)^T$, where $K_0 = \frac{\pi}{2}$, enclosed by the Fermi surfaces FS$_\pm$ in the presence of doping, as illustrated by the bulk energy spectrum in Fig. 2 (a) along the $k_z$ axis.

The band Hamiltonian $H_0$ has the symmetries required for realizing topological $\mathbb{Z}_2$ FSs. It preserves TRS, $\Theta h(k) \Theta^{-1} = h(-k)$, where $\Theta = is_y \otimes \tau_0 \circ K$ is the time-reversal operator satisfying $\Theta^2 = -1$, and $K$ is the complex conjugation operator. Furthermore, since $h(k)$ is invariant under $k_z \rightarrow -k_z$, this symmetry can be considered as the ‘mirror’ $M_z$, although it keeps the spin and orbital spaces invariant. $H_0$ also possesses 3D inversion symmetry, $\Pi h(k) \Pi^{-1} = h(-k)$, where $\Pi = \Gamma_1$. Combined with $M_z$, we have $P h(k_x, k_y, k_z) P^{-1} = h(-k_x, -k_y, k_z)$, where $P = i \Pi M_z$. The eigenvalues of $P$ of the states on the FSs along the $\hat{T}$-invariant line (the $k_z$ axis) are $s_n h_1(0, 0, k_z) = -s_n (m \cos k_z)$, which changes sign at the Dirac nodes. Hence, the two Fermi surfaces FS$_\pm$ are $\mathbb{Z}_2$ non-trivial by the Fu-Kane formula.

Now we consider the odd-parity pairing state $\tilde{\Delta}(q) = i \Delta_0 s_y \otimes \tau_x$, which describes spin-singlet and inter-orbital
L are the low-energy physics by projecting the gap function topological superconductor. The two emergent Dirac nodes at \( k = \pm k_d \) doubly degenerate bands cross at the two Dirac nodes at energy spectra along the \( k_z \)-direction. Within the gap are helical surface states on FS\(_-\), which are related to \( |\alpha_{+,\sigma}(q)\rangle \) by \( \hat{\Theta} \), are \( |\alpha_{-,\sigma}(q)\rangle = \left( u_q, -\frac{1}{\sqrt{2}} v_q, 0, -\frac{1}{\sqrt{2}} v_q \right)^T \) and \( |\alpha_{-,\sigma}(q)\rangle = \left( 0, -\frac{1}{\sqrt{2}} v_q^*, u_q^*, -\frac{1}{\sqrt{2}} v_q^* \right)^T \). Written in the above band basis, the projected gap function is

\[
\Delta^N(q) = \Delta_0 \sqrt{2} \left( \text{Re } u_q v_q^* - \text{Im } u_q v_q^* \right),
\]

which corresponds to triplet pairing with \( d^N(q) = \Delta_0 \sqrt{2} \sin \theta_q (\cos \phi_q, \sin \phi_q, \cos \phi_q)^T \). Locally, the gap function at constant \( k_z \) corresponds to that of a 2D helical topological superconductor. This description is not accurate globally, however. To determine the local gap function near the south pole, we perform the gauge transformation in Eq. (2) with transition matrix \( M_\alpha(q) = ie^{i(\phi_q + \frac{\pi}{2})}\sigma_z \), whose SU(2) part, \( G_\alpha(q) = e^{i(\phi_q + \frac{\pi}{2})}\sigma_z \), belongs to topological class (II). The gap function in gauge \( S \) is

\[
\Delta^S(q) = \Delta_0 \sqrt{2} \left( \text{Re } \tilde{u}_q \tilde{v}_q^* - \text{Im } \tilde{u}_q \tilde{v}_q^* \right),
\]

where \( \tilde{u}_q = \cos \frac{\theta_q}{2} e^{i\phi_q} \) and \( \tilde{v}_q = \sin \frac{\theta_q}{2} \). In this gauge, the Dirac string passes through the north pole and this gap function is an accurate local description in the vicinity of the south pole.

The local expressions for the gap function near the north and south poles satisfy, on a matrix level, \( \Delta^S(q) = \sigma_z \Delta^N(q) \sigma_z \). Therefore, a 2D momentum space slice labelled by \( k_z \) near the south pole has the same gap function as one near the north pole, but with the pseudospins reversed. Figs. 2 (c) and (d), which are momentum cuts near the north and south poles, respectively, illustrate this. Within the bulk gap are topological surfaces states with their \( \langle \sigma_z \rangle \) values shown. When we move from north to south, the pseudospins of the low-energy surface excitations are reversed.

The local gap functions can also be obtained using a non-singular gauge. Let \( |\chi_{+,\sigma}(q)\rangle = v_q^* |\alpha_{+,\sigma}(q)\rangle + u_q |\alpha_{+,\sigma}(q)\rangle \) and \( |\chi_{+,\sigma}(q)\rangle = v_q^* |\alpha_{+,\sigma}(q)\rangle + u_q |\alpha_{+,\sigma}(q)\rangle \), which are non-singular as they only consist of products of monopole harmonic functions with opposite monopole charges [45]. This gauge transformation corresponds to the change of basis matrix \( U(q) = e^{-i\theta_q \alpha \sigma \mu \alpha \mu} \), where \( \theta_q = (\sin \phi_q, \cos \phi_q, 0)^T \), and, using Eq. (9), we obtain for the \( d \)-vector

\[
d(q) = \Delta_0 \sqrt{2} \sin \theta_q \left[ \begin{array}{ccc}
\cos \phi_q & \sin \phi_q & 0 \\
\sin \phi_q & \cos \phi_q & 0 \\
0 & 0 & 1
\end{array} \right]
\]

and sewing matrix \( w_{\mu}(q + \pi \hat{\sigma}_\mu) = e^{-i\theta_q \alpha \sigma \mu \alpha \mu} \). The gap function matrix \( \Delta(q) \) is the same near the two poles. However, there is a twist in the basis: In the vicinity of the north pole, \( \chi_{+,\sigma}^\dagger(q) \simeq \delta_{+,\sigma}(q) \) and \( \chi_{+,\sigma}^\dagger(q) \simeq \delta_{+,\sigma}(q) \).
individual 2D slices labelled by trivial topology for this nodal phase arises by considering in our model and satisfies the same symmetries. The non-d\textsuperscript{2}conductors, whose order parameters are not obstructed. For 1 and 2, the pseudospins near the south pole are opposite those at the north pole.

We remark that this phase is fundamentally different from currently known TR invariant topological superconductors, whose order parameters are not obstructed. For example, consider a superconductor with order parameter \(\textbf{d}(\textbf{q}) = \frac{\alpha}{\sqrt{2}} \sin \theta_{\textbf{q}} (\cos \phi_{\textbf{q}}, \sin \phi_{\textbf{q}}) \hat{\textbf{T}}\). This is \(\mathbf{d}^\nu\) in our model and satisfies the same symmetries. The non-trivial topology for this nodal phase arises by considering individual 2D slices labelled by \(k_z\) and calculating the Fu-Kane invariant for each slice [41, 54]. Our system is also topological in this sense, but it has the further topological property that the order parameter is not well-defined over the FS, leading to the aforementioned topological twist in the quasiparticle spectrum.

Conclusion. – To conclude, we have studied a three-dimensional, TR symmetric nodal superconducting phase whose order parameter is topologically obstructed over the FS, preventing it from being defined globally. This arises when the Cooper pairing is in a triplet state and the FS, preventing it from being defined globally. This twist in the quasiparticle spectrum.

\[ \beta^\downarrow \theta_{\textbf{q}}(\cos \phi_{\textbf{q}}, \sin \phi_{\textbf{q}}) \hat{\textbf{T}}. \]

Between two FSs with non-trivial invariants, such as those in a \(\mathbb{Z}_2\) Dirac semimetal. When the \(\hat{T}\)-symmetry condition is imposed, the gap function must be described using two gauge patches and the transition function between the the gap functions in the two gauge patches corresponds to a non-contractible SO(3) rotation of the \(\textbf{d}\)-vector. As a result of the topological obstruction, the pseudospins of the surface states are opposite at the poles. The results were also discussed in the sewing matrix formalism, which selects a globally well-defined gauge at the expense of the \(\hat{T}\)-symmetry condition.

Acknowledgment. – C.S. and Y.L. are supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, Grant No. DE-SC0019331. This work was supported in part by the Alfred P. Sloan Research Fellowships.
[46] A. Schnyder, S. Ryu, A. Furusaki, and A. Ludwig, Phys. Rev. B 78, 195125 (2008).
[47] C. Sun, S.-P. Lee, and Y. Li, arXiv preprint arXiv:1909.04179 (2019).
[48] Y. Li, arXiv preprint arXiv:2001.05984 (2020).
[49] E. Muoz, R. Sotto-Garrido, and V. Jurii, “Monopole versus spherical harmonic superconductors: Topological repulsion and stability,” (2020), arXiv:2007.12190 [cond-mat.supr-con].
[50] E. Bobrow, C. Sun, and Y. Li, Phys. Rev. Research 2, 012078 (2020).
[51] L. Fu and C. L. Kane, Phys. Rev. B 74, 195312 (2006).
[52] C. Fang, L. Lu, J. Liu, and L. Fu, Nature Physics 12, 936 (2016).
[53] T. Morimoto and A. Furusaki, Phys. Rev. B 89, 235127 (2014).
[54] A. P. Schnyder and S. Ryu, Phys. Rev. B 84, 060504 (2011).
[55] S. Ryu, C. Mudry, H. Obuse, and A. Furusaki, New Journal of Physics 12, 065005 (2010).
SUPPLEMENTAL MATERIALS

I. SU(2) WILSON LOOP

In this supplementary material, the equivalence between the two \( Z_2 \) invariants defined in the main text is established. The first invariant, \( \delta_0 \), is the relative sign between the SU(2) transition matrices at points related by \( \hat{T} \)-symmetry [20],

\[
G(q) = \delta_0 G(q + \pi \phi_q). ~ (S1)
\]

The second is the Fu-Kane formula in Eq. (5) [52],

\[
\delta = \text{Pf} \hat{w}_+ (\theta_q = 0) \text{Pf} \hat{w}_+ (\theta_q = \pi), ~ (S2)
\]

which characterizes the inability to select the SU(2) part of \( \hat{T} \) to be \( i\sigma_y \) globally. As discussed in the main text, the two Fermi surfaces belong to the same topological class, so we will henceforth focus on FS\(_+\) and omit the + subscript for notational convenience.

Following Ref. [20], the two \( Z_2 \) invariants can be expressed as an SU(2) Wilson loop. In a gauge where the eigenstates are non-singular, \( |\chi_a(q)\rangle \equiv \chi_a^T(q)|0\rangle \), it is possible to define the U(2) Berry connection \( A_{ab}(q) = i\langle \chi_a(q)|\nabla_q|\chi_b(q)\rangle \) over the entire FS. It is useful to decompose \( A \) into U(1) and SU(2) parts: \( A = A_{U(1)} + A_{SU(2)} \), where \( A_{U(1)} \) and \( A_{SU(2)} \) are the traceful and traceless parts of \( A \), respectively. The central object connecting the two definitions for the \( Z_2 \) invariant is the Wilson loop [20, 51]

\[
W[C] = \frac{1}{2} \text{Tr} \mathcal{P} \exp \left[ i \oint_C dq \cdot A_{SU(2)}(q) \right], ~ (S3)
\]

where \( \mathcal{P} \) is the path-ordering operator and \( C \) is the \( \hat{T} \)-invariant loop in Fig. S1, which is separated into four segments \( C_{1-4} \). The Wilson loop is gauge invariant as a result of the trace.

![Figure S1](https://example.com/figure_s1.png)

**FIG. S1.** The Fermi surface FS\(_+\) consists of two gauge patches, \( N \) (red) and \( S \) (blue), with overlap \( N \cap S \) (green). The \( \hat{T} \)-invariant Wilson loop \( C \), which is separated into four segments \( C_{1-4} \), is a great circle that passes through the north and south poles. For concreteness the meridians are taken to be at \( \phi_q = 0, \pi \).

To evaluate the Wilson loop, consider the unitary infinitesimal propagator [55]

\[
K_{ab}(q_2, q_1) \equiv \langle \chi_a(q_2)|\chi_b(q_1)\rangle = [e^{i\sigma_y A_{SU(2)}(q_2)}]_{ab}, ~ (S4)
\]

where \( dq = q_2 - q_1 \). As a result of \( \hat{T} \)-symmetry, it satisfies the sewing condition \( K(q_1 + \pi \hat{\phi}_q, q_2 + \pi \hat{\phi}_q) = w(q_1)K^T(q_2, q_1)w^\dagger(q_2) \). When the propagator is decomposed into U(1) and SU(2) parts, \( K(q_1, q_2) = e^{i\sigma_y A_{SU(2)}(q)} K(q_1, q_2), \) where \( U(q_2, q_1) = e^{i\sigma_y A_{SU(2)}(q)} \), the SU(2) part of the propagator satisfies the corresponding sewing condition

\[
\tilde{K}(q + \pi \hat{\phi}_q, q_2 + \pi \hat{\phi}_q) = \tilde{w}(q_1)\tilde{K}^T(q_2, q_1)\tilde{w}^\dagger(q_2). ~ (S5)
\]

Here \( \tilde{w}(q) \) is the SU(2) part of the sewing matrix, as defined in the main text. The Wilson loop can be constructed from the infinitesimal propagators by

\[
W[C] = \frac{1}{2} \text{Tr} \tilde{K}_4 \tilde{K}_3 \tilde{K}_2 \tilde{K}_1, ~ (S6)
\]

where the propagators for the four segments, \( C_{1-4} \), are

\[
\begin{align*}
\tilde{K}_1 &\equiv \prod_{n=1}^{N} \tilde{K}_n \left( \frac{\pi}{2} + n\delta\theta_q, \frac{\pi}{2} + (n-1)\delta\theta_q \right), \\
\tilde{K}_2 &\equiv \prod_{n=1}^{N} \tilde{K}_0 \left( \pi - n\delta\theta_q, \pi - (n-1)\delta\theta_q \right), \\
\tilde{K}_3 &\equiv \prod_{n=1}^{N} \tilde{K}_0 \left( \frac{\pi}{2} - n\delta\theta_q, \frac{\pi}{2} - (n-1)\delta\theta_q \right), \\
\tilde{K}_4 &\equiv \prod_{n=1}^{N} \tilde{K}_n \left( n\delta\theta_q, (n-1)\delta\theta_q \right).
\end{align*}
\]

Here \( \delta\theta_q = \frac{\pi}{N} \) and we use the notation \( \tilde{K}_{\phi_q}(\theta_q, q_1) = \tilde{K}(q_1, q_2), \) where \( q_1 = (\theta_q, \phi_q) \) and \( q_2 = (\theta_{2q}, \phi_{2q}) \). The sewing condition gives the constraints, \( \tilde{K}_1 = \tilde{w}(\theta_q = 0, \pi)\tilde{K}_2 \tilde{w}^\dagger(\theta_q = \pi/2) \) and \( \tilde{K}_4 = \tilde{w}(\theta_q = \pi/2)\tilde{K}_3 \tilde{w}^\dagger(\theta_q = 0) \). Using \( \tilde{w}(\theta_q = 0, \pi) = \text{Pf} \tilde{w}(\theta_q = 0, \pi) = 0 \) and the identity \( \sigma_y F^T \sigma_y = F^\dagger \) for any SU(2) matrix \( F \), the Wilson loop reduces to the Fu-Kane invariant, \( W[C] = \delta \).

The Wilson loop \( W[C] \) is also equal to the invariant \( \delta_0 \). To arrive at the appropriate form for \( W[C] \), perform for the propagators in the segments \( C_3 \) and \( C_4 \) a gauge transformation to \( |\alpha_a(q)\rangle = \sum_b |\alpha_b(q)\rangle U_{ba}(q), \) where \( |\alpha_a(q)\rangle \equiv \tilde{\alpha}_a^T(q)|0\rangle \) are states smooth over \( N \) and satisfy the \( \hat{T} \)-symmetry condition, Eq. (1). Under this gauge transformation, the propagators transform as \( \tilde{K}(q_2, q_1) = U_{\phi}^T(q_2) K_N(q_2, q_1) U_{\phi}(q_1), \) where \( U_{\phi}(q) \) and \( K_N^{\phi}(q_2, q_1) \) are the SU(2) parts of \( U(q) \) and \( K_{\phi}(q_2, q_1) \equiv \langle \alpha_a(q)|\alpha_b(q)\rangle \), respectively. In this gauge, the \( \hat{T} \)-symmetry condition is enforced, hence Eq. (S5) simplifies to \( \tilde{K}_N(q_1 + \pi \hat{\phi}_q, q_2 + \pi \hat{\phi}_q) = [K_N^{\phi}(q_2, q_1)]^\dagger. \)
Consequently, the propagators $\tilde{K}^N$ in the entire segment $C_3 \cup C_4$ cancel and $\tilde{K}_4 \tilde{K}_3 = \tilde{U}^\dagger(\theta_q = \pi/2, \phi_q = \pi)\tilde{U}(\theta_q = \pi/2, \phi_q = 0)$. Similarly, the propagators in the segments $C_1$ and $C_2$ are evaluated in the gauge $S$ by performing the gauge transformation $|\chi_a(q)\rangle = \sum_b |\beta_{b}(q)\rangle V_{ba}(q)$, where $|\beta_{b}(q)\rangle \equiv \beta^\dagger_{b}(q)|0\rangle$. By the same argument, only the gauge transformations at the end points contribute and $\tilde{K}_2 \tilde{K}_1 = \tilde{V}^\dagger(\theta_q = \pi/2, \phi_q = 0)\tilde{V}(\theta_q = \pi/2, \phi_q = \pi)$. The change of basis matrices $U(q)$ and $V(q)$ are related to the transition matrix by $G(q) = \tilde{V}(q)\tilde{U}^\dagger(q)$. Hence, $W[C] = \frac{1}{2} \text{Tr}[G(\theta_q = \pi/2, \phi_q = \pi)G^\dagger(\theta_q = \pi/2, \phi_q = 0)] = \delta_0$. This establishes that the two invariants, $\delta_0$ and $\delta$, are equal to the Wilson loop $W[C]$. 