Nodal lines and nodal loops in non-symmorphic odd-parity superconductors

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We discuss the nodal structure of odd-parity superconductors in the presence of non-symmorphic crystal symmetries, both with and without spin-orbit coupling, and with and without time reversal symmetry. We comment on the relation of our work to previous work in the literature, and also the implications for unconventional superconductors such as UPt$_3$.

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I. INTRODUCTION

Power-law temperature dependences of certain physical properties in heavy electron superconductors that were discovered in the 1980s indicated the possible presence of nodes of the superconducting order parameter that form lines on the Fermi surface. This motivated a study by Blount[2] where he showed that in the presence of spin-orbit coupling, one would not expect line nodes for an odd-parity order parameter: the constraint of having all three components of the triplet vanish can happen at most at points on the Fermi surface. This was an issue when an odd-parity order parameter was proposed to explain experimental data in UPt$_3$[3] which was consistent with later phase sensitive Josephson tunneling measurements[4]. In 1995, though, one of the authors found a possible solution to this problem, by showing that there is a counter example to Blount’s theorem for non-symmorphic odd-parity superconductors (UPt$_3$ being such an example given its P6$_3$/mmc space group)[5].

By explicit construction of the pair wave functions, it was found that on the zone face, $k_z = \pi/c$, all components of the triplet belonged to the same group representation (as opposed to what happens on the $k_z = 0$ zone plane), meaning that for the proposed E$_{2u}$ symmetry, line nodes are indeed possible (two of the Fermi surfaces of UPt$_3$ intersect this zone face). This was a consequence of the non-symmorphic phase factors associated with the c-axis (which is a screw axis for this space group). These considerations also potentially apply to other superconductors. For instance, UBe$_{13}$ has the non-symmorphic space group Fm$\overline{3}c$.

In 2009, a more rigorous treatment of this problem for the general non-symmorphic case was formulated by us based on group theoretical arguments[6]. Very recently, this problem has been revisited by Yanase[7] and Kobayashi et al.[8]. The former found that the nodal ‘lines’ actually reconstruct to form nodal ‘loops’ (called ‘rings’ in the latter) which, as we demonstrate here, shrink to zero as the ratio of the superconducting gap to the spin-orbit interaction increases. This is discussed in greater detail in Section III. The latter also discussed the mirror eigenvalues associated with these nodal loops, as well as contrasted the group theoretical and topological approaches to this problem. It is our purpose here to clarify matters by a general group theoretical approach that in addition generalizes our previous work to the case where spin-orbit interactions are absent, and also to the case of time reversal symmetry breaking. We also consider the effect of glide-plane symmetries, and find that these do not protect line nodes as do the screw-axis symmetries.

II. GROUP THEORY

The nodal structure of superconducting order parameters can be understood from representations of the symmetry group of the underlying crystal. The absence of certain representations on high-symmetry planes or lines in the Brillouin zone implies the presence of line or point nodes of the Cooper-pair wave function, respectively, in cases where the Fermi surface intersects these planes or lines. Representations of the superconducting order parameter in symmorphic crystals are readily found from the underlying point-group symmetries[9]. Non-symmorphic crystals, however, contain symmetries which consist of the combined operation of point-group elements with translations by fractions of a lattice vector. These non-primitive translations generate additional phase factors which have to be accounted for in the derivation of the Cooper-pair representations. Indeed, these phase factors may conspire in a way to exclude some of the symmetry-allowed representations on high symmetry planes, implying the possibility of new symmetry-enforced line nodes of the order parameter which are absent in symmorphic crystals[6,7].

A convenient way to derive space-group representations of the Cooper-pair wave function is to construct anti-symmetrized products of the irreducible single-particle space-group representations[10,11] as we discuss next.
A. Induced Cooper-pair representations

Consider a centrosymmetric crystal generated by a non-symmorphic space-group. In the following, we denote space-group elements by \((g, t)\), where \(g\) refers to the point-group operation and \(t\) accounts for possible non-primitive lattice translations, e.g. \((I, 0)\) is the inversion symmetry, etc. Our focus here is on line nodes in odd-parity superconductors protected by non-symmorphic symmetries. We therefore concentrate on odd-parity representations of the Cooper-pair wave function at Brillouin-zone points \(k\) belonging to symmetry planes of non-symmorphic symmetry operations. Specifically, we consider symmetry planes \(k_\perp = 0, \pi\) of a glideoperation \((\sigma_z, t_\perp)\) and the combined action of inversion and two-fold screw axis, \((2_\perp, t_\perp)(I, 0)\) (from now on, we set the lattice constant to unity). Here and in the following, \(2_\perp\) denotes the two-fold rotation around the \(z\)-axis, \(\sigma_z\) is reflection in the \(z\)-plane, and \(t_\perp/\sigma\) is half a primitive translation along/perpendicular to the \(z\)-direction.

One can construct representations of the Cooper-pair wave function from the single-particle representations \(\gamma_k\) of symmetry-operations \(m \in G_k\) leaving \(k\) invariant (the “little group”).\(^{[12]}\) To this end, one induces representations \(P^-\) of the anti-symmetrized Kronecker-product with vanishing total momentum (modulo a reciprocal lattice vector)\(^{[11,13]}\)

\[
\chi(P^-(m)) = \chi(\gamma_k(m))\chi(\gamma_k(\mathbf{I}m\mathbf{I})),
\]

\[
\chi(P^-(\mathbf{I}m)) = -\chi(\gamma_k(\mathbf{I}m\mathbf{I}m)),
\]

where \(\chi\) are the characters of the representation and for notational convenience we introduced \(\mathbf{I} \equiv (I, 0)\). In the presence of the spin-orbit interaction, the above equations characterize the pseudo-spin-triplet components of the Cooper-pair wave function. In the absence of spin-orbit, spin-rotational symmetry is conserved and they account for the Cooper pair’s orbital degree of freedom of a spin-triplet state.

Single-particle representations \(\gamma_k\) entering Eqs. (1), (2) are double- or single-valued, depending on the presence of the spin-orbit interaction. Time-reversal symmetry \(\theta\) can moreover induce extra degeneracies. These are detected by Herring’s criterion\(^{[11,13]}\) and taken into account by passing to the corresponding co-representations (see Appendix A for details). We next apply the outlined procedure to construct Cooper-pair representations for the symmetries of interest.

B. Two-fold screw axis

Consider first the presence of a two-fold screw symmetry \((2_\perp, t_\perp)\) along the \(z\)-axis. Line nodes can be enforced on the symmetry planes \(k_\perp = 0, \pi\) characterized by the little group \(G_k = \{(E, 0), (\sigma_z, t_\perp)\}\). Notice that in spite of its non-primitive translation vector \((\sigma_z, t_\perp) = (2_\perp, t_\perp)\mathbf{I}\) is a symmorphic operation since the former can be removed by redefinition of the spatial origin (that is, it is a mirror plane, not a true glide plane). We next induce representations in the described manner, i.e. by defining characters for the symmetry operations in \(G_k \cup I G_k = \{(E, 0), (\sigma_z, t_\perp), (I, 0), (2_\perp, t_\perp)\}\).

Recalling the multiplication rule for non-symmorphic group elements\(^{[12]}\) \((g_1, t_1)(g_2, t_2) = (g_1g_2, t_1 + g_1t_2)\), it is verified that \(I(\sigma_z, t_\perp)I = e^{-ikz}(\sigma_z, t_\perp)\). We can thus simplify characters in Eqs. (1), (2) for the symmetry planes of interest as summarized in Table I. From this table we then read off irreducible components of the Cooper-pair representations given in Table II. Notice that the second column in Tables I and II determines the mirror eigenvalue of the Cooper pair. We are thus left with the task of finding characters in the second and fourth column which depend on the underlying symmetries.

In the presence of the spin-orbit interaction, \(\gamma_k\) are double-valued with purely imaginary eigenvalues. That is, \(\chi(\gamma_k(\sigma_z^2, 0)) = -d\) and \(\chi(\gamma_k(\sigma_z, t_\perp)) = \pm id\) with \(d\) the dimension of \(\gamma_k\). Time-reversal symmetry may induce extra degeneracies. Applying Herring’s criterion one indeed detects (Kramers) degeneracies on both symmetry planes. That is, \(d = 2\) and one has to consider the corresponding double-valued co-representations (see Appendix A for details). If time-reversal symmetry is broken, \(\gamma_k\) are one-dimensional. In the absence of the spin-orbit interaction, \(\gamma_k\) only account for the orbital degree of freedom, i.e. are single-valued. That is, \(\chi(\gamma_k(\sigma_z^2, 0)) = d\) and \(\chi(\gamma_k(\sigma_z, t_\perp)) = \pm d\). Herring’s criterion then signals degeneracies induced by time-reversal symmetry on the Brillouin zone face \(k_\perp = \pi\). The latter are known as “sticking of bands” induced by a two-fold screw axis\(^{[11,13]}\), and one has to pass to the single-valued co-representation (see again Appendix A for details). When time-reversal symmetry is broken, \(\gamma_k\) are again one-dimensional.

All characters of the induced representations are summarized in Table I.

\[
\begin{array}{cccc}
\hline
k_\perp & (E, 0) & (\sigma_z, t_\perp) & (I, 0) & (2_\perp, t_\perp) \\
\hline
k_\perp = \pi & d^2 - \chi^2((\sigma_z, t_\perp)) & -d & \chi(\sigma_z^2, 0) \\
(2_\perp, t_\perp) & d^2 & -d & -\chi(\sigma_z^2, 0) \\
\hline
\end{array}
\]

TABLE I: Character table for representations \(P^-\) of anti-symmetrized Kronecker deltas induced by single-particle representations of dimension \(d\) on the high-symmetry planes. For notational convenience, we suppress \(\gamma_k\).

\[
\begin{array}{cccc}
\hline
(E, 0) & (\sigma_z, t) & (I, 0) & (2_\perp, t) \\
\hline
A_0 & 1 & 1 & 1 & 1 \\
A_u & 1 & -1 & -1 & 1 \\
B_g & 1 & -1 & 1 & -1 \\
B_u & 1 & 1 & -1 & -1 \\
\hline
\end{array}
\]

TABLE II: Character table for the irreducible representations of the Cooper-pair wave function on high symmetry planes of a screw-axis/glide-plane \((t = t_{\perp/\sigma}\) for a screw-axis/glide-plane). The second column determines the mirror eigenvalue of the Cooper pair.
The last four rows apply in the absence of the spin-orbit interaction. The indicated representations then classify the orbital part of the pair wave function. This is combined with one of the three symmetric spin-triplet states to guarantee overall anti-symmetry of the pair wave function. In the absence of band degeneracies, representations are thus one-dimensional, as in the last three rows, allowing for symmetry protected line nodes on both symmetry planes. In the presence of time-reversal symmetry, the two-fold screw axis induces, however, sticking of bands on the Brillouin zone face\(^\text{[33]}\) (fifth row). One thus finds four allowed representations and both mirror eigenvalues are realized. In the absence of both the spin-orbit interaction and time reversal breaking, symmetry-protected line-nodes are thus possible on the basal plane but do not exist on the Brillouin zone face. The difference from the first two lines of this Table is that this sticking of bands allows the formation of interband pairs in this case\(^\text{[33]}\). The interband pairs are odd in the band index, implying that the intra-orbital part of the Cooper pair wave function is even to guarantee overall odd-parity (that is, they have opposite mirror eigenvalues to the intraband pairs). We will return to this point below. In the absence of time-reversal symmetry, protected line nodes can appear on both symmetry planes, independent of the spin-orbit interaction. Finally, we note that for time reversal symmetry breaking, the inversion of the sign of the Cooper-pair mirror eigenvalue of one-dimensional representations in the presence (third and fourth rows) and absence (seventh and eighth rows) of the spin-orbit interaction is readily related to the double- and single-valuedness of the representations.

### C. Glide plane

Consider next a glide-plane symmetry \((\sigma_z, t_\sigma)\), where without loss of generality we can assume \(t_\sigma\) parallel to the \(x\)-axis. The little group on the symmetry planes \(k_z = 0\), \(\pi = G_k = \{(E, 0), (\sigma_z, t_\sigma)\}\) and we induce representations for the symmetry operations in \(G_k \cup \Sigma G_k = \{(E, 0), (\sigma_z, t_\sigma), (I, 0), (2z, t_\sigma)\}\). Here \((2z, t_\sigma)\) in spite of its non-primitive translation is a symmorphic operation (again the translation can be removed by redefinition of the spatial origin). Using the commutation relation \(I(\sigma_z, t_\sigma) = e^{-ik_z}(\sigma_z, t_\sigma)\), characters of the induced representations can be simplified, as shown in Table\(\text{[IV]}\). The induced representations are identical on both symmetry planes.

| SO | TRS | BZ plane | irreducible components |
|----|-----|----------|------------------------|
| yes | yes | \(k_x = \pi\) | \(P^- = A_y + 3B_u\) |
|     |     | \(k_x = 0\) | \(P^- = A_y + B_u + 2A_u\) |
| yes | no  | \(k_x = \pi\) | \(P^- = B_u\) |
|     |     | \(k_x = A_u\) | \(P^- = B_u\) |
| no  | yes | \(k_x = \pi\) | \(P^- = A_y + B_u + 2A_u\) |
|     |     | \(k_x = 0\) | \(P^- = B_u\) |
| no  | no  | \(k_x = \pi\) | \(P^- = A_u\) |
|     |     | \(k_x = 0\) | \(P^- = B_u\) |

**TABLE III:** Decompositions of Cooper-pair representations into their irreducible components. Here \(g\) and \(u\) denote the even- and odd-parity representations and \(A_y/B_u\) and \(B_y/A_u\) are representations which are even and odd under reflection in the symmetry plane (i.e., mirror eigenvalues \(\pm 1\)), respectively. The results depend on the presence of time-reversal symmetry (TRS) and the spin-orbit interaction (SO).
nodes typically form as loops. Only two-fold screw axes can protect line nodes in odd-order time-reversal symmetry and the spin-orbit interaction, symmetry-protected line nodes can occur on both even/odd under reflection in the symmetry plane. In the absence of time-reversal symmetry (TRS) and the spin-orbit interaction, on the other hand, all single-particle representations are one-dimensional, independent of time-reversal symmetry.

All characters of the induced representations are summarized in Appendix [A] Table[V] shows the decompositions of the resulting Cooper-pair representations into irreducible components of Table[I]. If the spin-orbit interaction and time-reversal symmetry are both present, all odd-parity representations are allowed on both planes. That is, glide-plane symmetries do not provide us with counter examples to Blount’s theorem. In the absence of either time-reversal symmetry or the spin-orbit interaction, symmetry-protected line nodes can occur on both symmetry planes.

Our discussion so far has shown that in the presence of time-reversal symmetry and the spin-orbit interaction, only two-fold screw axes can protect line nodes in odd-parity superconductors. Next, we discuss that these line nodes typically form as loops.

### III. NODAL STRUCTURE OF ODD-PARITY SUPERCONDUCTORS

As pointed out by Yanase[5], the nodal lines discussed above in the \( k_z = \pi \) zone face actually reconstruct to form nodal loops in the case of UPt3. The latter are, in contrast to line nodes, contractible, i.e. they continuously shrink to zero as the ratio of the superconducting gap to the spin-orbit interaction increases. The formation of these nodal loops can be understood from the results of Section II. In particular, along the \( A-L \) lines of this zone face, the spin-orbit interaction vanishes, leading to band sticking (this band sticking effect has been seen in UPt3 from breakdown orbits in deHaas-vanAlphen measurements[23]). This means that interband pairs can form at these sticking points on the Fermi surface, and since they have opposite mirror eigenvalues, they are allowed representations for the case where the intraband pairs are not allowed. This leads to a gapping of the Fermi surface at these points, thus converting the nodal lines to nodal loops, as we illustrate in Figs. 1 and 2. As the order parameter increases, these nodal loops will eventually shrink to zero, leading to a topological transition (Fig. 1c). In Ref. [24] topological arguments are presented (following earlier work[25]) that confirm the group theoretical ones. There, a claim was made that the topological arguments are more general than the group theory ones, but in fact they are equivalent. In particular, as we showed in Section II, in the presence of time rever-
Degeneracies induced by $\theta$ should pass from the representations to corresponding co-representations. This will be addressed in the consequences of the effects discussed here on potential topological surface states. This work was supported by the Materials Sciences and Engineering Division, Basic Energy Sciences, Office of Science, US Dept. of Energy. T. M. acknowledges financial support by Brazilian agencies CNPq and FAPERJ.

Appendix A: Herring’s criterion and co-representations

As stated in the main text, time-reversal symmetry $\theta$ can induce additional degeneracies. In this case, one should pass from the representations to corresponding co-representations of the magnetic group $\mathcal{G}_k = \mathbf{G}_k + i\mathbf{B}G_k$. Degeneracies induced by $\theta$ can be detected by Herring’s criterion from the sum of characters:

$$
\sum_{\mathbf{B} \in G_k} \chi (\gamma_k(i\mathbf{B})^2) = \begin{cases} +|G_k| & \text{case (a)} \\ -|G_k| & \text{case (b)} \\ 0 & \text{case (c)}. \end{cases} \quad (A1)
$$

Here $|G_k|$ is the order of the little group. In case (a) no degeneracies are induced, while (b) and (c) indicate the presence of degeneracies. The latter are accounted for by passing to co-representations $\gamma_k \mapsto \Gamma_k \equiv (\gamma_k \gamma_k^*)$, where $\gamma_k(m) = \gamma_k(m)$ in case (b) and $\gamma_k^*(m) = \gamma_k^*(i\mathbf{B})^{-1} m i\mathbf{B}$ in case (c), respectively, with $'*$' the complex conjugation. We next consider the cases of interest.

**Two-fold screw axis:** In presence of the spin-orbit interaction, the sum of characters for double-valued representations reads

$$
\chi ([i\mathbf{B}(E, 0)^2] + \chi ([i\mathbf{B}(\sigma_z,t_2)^2]) = -\chi ((E, 0)) - e^{ik_x} \chi ((\sigma_z^2, 0)) = -1 + e^{ik_z}, \quad (A2)
$$

where we used that $\theta_{g1}\theta_{g2} = -g_1g_2$. For double valued co-representations on the basal-plane (case (c)), we then employ $\gamma_k^*(\sigma_z, t_2) = \gamma_k^*(i\mathbf{B})^{-1}(\sigma_z, t_2) i\mathbf{B}$, for single-valued representations, on the other hand, $\theta_{g1}\theta_{g2} = g_1g_2$ and

$$
\chi ([i\mathbf{B}(E, 0)^2] + \chi ([i\mathbf{B}(\sigma_z,t_2)^2]) = \chi ((E, 0)) + e^{ik_x} \chi ((\sigma_z^2, 0)) = 1 + e^{ik_z}. \quad (A3)
$$

For the single-valued co-representation on the Bril-louin zone face (case (c)), we use that $\gamma_k((\sigma_z, t_2)) = -\gamma_k^*(\sigma_z, t_2)$.

**Glide-plane symmetry:** In presence of the spin-orbit interaction

$$
\chi ([i\mathbf{B}(E, 0)^2] + \chi ([i\mathbf{B}(\sigma_z, t_\sigma)^2]) = -\chi ((E, 0)) + \chi ((\sigma_z^2, 0)) = 0, \quad (A4)
$$

and for the double valued co-representations (case (c)), we then employ $\gamma_k((\sigma_z, t_\sigma)) = \gamma_k^*(i\mathbf{B})^{-1}(\sigma_z, t_\sigma) i\mathbf{B} = e^{ik_x} \gamma_k^*(\sigma_z, t_2)$, i.e. $\Gamma_k((\sigma_z, t_\sigma)) = \pm e^{ik_x} / (-i)$. In the absence of the spin-orbit interaction

$$
\chi ([i\mathbf{B}(E, 0)^2] + \chi ([i\mathbf{B}(\sigma_z, t_\sigma)^2]) = \chi ((E, 0)) + \chi ((\sigma_z^2, 0)) = 2. \quad (A5)
$$

Appendix B: Irreducible representations of the Cooper-pair wave function

We summarize the characters of induced representations in the case of a two-fold screw axis (Table V) and
a glide-plane symmetry (Table VII). The decompositions of Cooper-pair representations into their irreducible components are done using the character table for the zero-momentum representations of the Cooper-pair wave function defined in Table III in the main text.

| SO | TRS | BZ plane | \((E, 0) \ (\sigma_z, t_2) \ (I, 0) \ (2z, t_2)\) |
|----|-----|----------|---------------------------------------------|
| yes | yes | \(k_z = \pi\) | 4 4 \(-2\) \(-2\) |
| yes | no  | \(k_z = \pi\) | 1 1 \(-1\) \(-1\) |
| no  | yes | \(k_z = \pi\) | 4 0 \(-2\) 2 |
| no  | no  | \(k_z = \pi\) | 1 1 \(-1\) \(-1\) |

TABLE VII: Character table for representations \(P^-\) of anti-symmetrized Kronecker deltas on symmetry planes induced by single- or double-valued (co-)representations.

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