Odd Parity and Line Nodes in Heavy Fermion Superconductors

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Abstract

Group theory arguments have demonstrated that a general odd parity order parameter cannot have line nodes in the presence of spin-orbit coupling. In this paper, it is shown that these arguments do not hold on the $k_z = \pi/c$ zone face of a hexagonal close packed lattice. In particular, three of the six odd parity representations vanish identically on this face. This has potential relevance to the heavy fermion superconductor $UPt_3$.

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The symmetry of the order parameter of heavy fermion superconductors is still an unresolved issue after over a decade’s worth of work. Even the parity of the order parameter has not been determined. At an early stage, though, group theory arguments were given that limited the number of possibilities for the order parameter. In particular, Blount showed that a general odd parity order parameter would not have line nodes in the presence of spin-orbit coupling. Since experimental evidence in many heavy fermion superconductors, especially $UPt_3$, point to the presence of line nodes in the order parameter, most theoretical models assume an even parity order parameter. In this paper, a review of this argument is given and then a particular example is analyzed where this argument fails. This example is the $k_z = \pi/c$ zone face of a hexagonal closed packed lattice, such as $UPt_3$, where it will be shown that three of the six odd parity representations vanish.

In this paper, only the case of a hexagonal close packed lattice is treated. The above argument of Blount is most easily illustrated by the use of basis functions, a complete set of which were recently published by Yip and Garg (Blount’s argument, though, is general and does not depend on the use of basis functions). For instance, consider the $E_{1u}$ ($\Gamma^-$) representation. Basis functions at the p-wave level are $k_z(\hat{x} \pm i\hat{y})$ and $(k_x \pm ik_y)\hat{z}$ where $\hat{x}$, $\hat{y}$, and $\hat{z}$ are basis functions for $S=1$. Although the first function does have a line of nodes, in the presence of spin-orbit, the two functions will be mixed with one another (since $S_z$ is no longer a good quantum number). Therefore, in general, only point nodes can occur.

Most odd parity models that have been discussed in connection with $UPt_3$ ignore this mixing effect (an example being the $E_{2u}$ model of Norman and Sauls where only the $S_z=0$ component is kept). An exception was a recent model of Norman which treated the strong spin-orbit limit of on-site pairing. In this case, it was found that the $\Gamma^-_6$ ($E_{2u}$) pair state vanished on the $k_z = \pi/c$ zone face. The question is whether this result is specific or can be generalized.

The first question to address is how Blount’s argument was circumvented in this case. To do this requires an analysis of single particle wavefunctions. The f electron part of the single particle wavefunctions is a linear combination of $J=5/2$ functions (where $J$ denotes the total angular momentum). In the case of a hexagonal close packed lattice, there are two f atoms per primitive cell (separated by a non-primitive translation vector). Therefore, the wavefunction is of the form $A^\mu_{i\mu}|\mu>\nu$ where $n$ is a band index, $\mu$ a basis function (-5/2,-3/2,-1/2,1/2,3/2,5/2), and $\nu$ a site index (1,2). Consider the two symmetry planes $k_z = 0$ and $k_z = \pi/c$ (these are the only symmetry planes perpendicular to the c axis, and are of interest for $UPt_3$ since line nodes perpendicular to c have been inferred experimentally). For a particular site, $i$, only functions differing by two units of angular momentum can mix. This occurs since these planes are mirror planes relative to the operation $z \to -z$ ($\sigma_h$) and the functions -5/2,-1/2,3/2 transform as -i and -3/2,1/2,5/2 as +i under this operation. Thus, for a particular site, the coefficients of either -5/2,-1/2,3/2 or -3/2,1/2,5/2 vanish. For the $k_z = 0$ case, the $a_{\mu}$ coefficients which are zero on one site are also zero on the other site, but for the $k_z = \pi/c$ case, they are “staggered” (that is, if -5/2,-1/2,3/2 are zero on site 1, then -3/2,1/2,5/2 will be zero on site 2). This difference occurs since the factor $e^{ik_z}$ will introduce a relative phase between the two sites of 1 for $k_z = 0$ and -1 for $k_z = \pi/c$.
corresponding to either even or odd parity must be constructed. This was first considered in
the presence of spin-orbit by Anderson. At a general \( \vec{k} \), there are two Kramers degenerate
states labeled \( k \) and \( PTk \) where \( P \) is the parity operator and \( T \) the time reversal operator,
corresponding to up spin and down spin in the spin only case. The analogous states at \(-k \)
can be labeled as \( Pk \) and \( Tk \). The even parity combination is then \( k, Tk - PTk, Pk \) and is a
pseudo-spin singlet (corresponding to \( S = 0 \) in the spin only case). For odd parity, there are
three pseudo-spin combinations: \( k, Pk \) and \( PTk, Tk \) and \( k, Tk + PTk, Pk \) (corresponding to
\( S = 1 \) in the spin only case). These are conveniently relabeled as a vector, \( \vec{d} \), with the above
three states corresponding to \(-d_x + id_y, d_x + id_y, \) and \( d_z \). Finally, to consider the full effect
of the space group on the order parameter, it is necessary to analyze the pair wavefunction
in real space. The cases of electrons on the same site, electrons separated by a non-primitive
lattice vector, and electrons separated by a primitive lattice vector have been treated by
Appel and Hertel (it is from this work that the arguments below will be obtained). By
construction, then, if something is proved for these three cases, then it is true for the general
pair wavefunction since all atom sites are connected by either a primitive or non-primitive
lattice vector.

For on-site pairs, three of the six possible odd parity representations, labeled even \( z \)
representations (\( \Gamma_1^-, \Gamma_2^-, \Gamma_5^- \)), involve states with even \( M_J \), the other three, labeled odd \( z \)
representations (\( \Gamma_3^-, \Gamma_4^-, \Gamma_6^- \)), involve states with odd \( M_J \). This along with the statements
in the above two paragraphs allows one to trivially conclude the following (remembering that
the operator \( P \) interchanges sites 1 and 2 in the unit cell, whereas the operator \( T \) interchanges \( \mu \)
and \(-\mu \)). For \( k_z = 0 \), using the relations satisfied by the single particle wavefunctions,
combinations like \( k, Pk \) are non-vanishing only for odd \( M_J \) states whereas combinations
like \( k, Tk \) are non-vanishing only for even \( M_J \) states. Thus, for even \( z \) representations, \( d_x \)
and \( d_y \) vanish, whereas for odd \( z \) representations, \( d_z \) vanishes. These are the arguments
appropriate to basis functions as discussed in the first part of this paper since such basis
functions involve expansions about \( \vec{k} = 0 \). The situation, though, changes for the \( k_z = \pi/c \)
case given the “staggering” of the single particle wavefunctions discussed above. In this case,
only even \( M_J \) states are non-vanishing for both \( k, Pk \) and \( k, Tk \) combinations. Therefore,
for even \( z \) representations, all three pseudo-spin components are in general non-zero on this
face, whereas for odd \( z \) representations, all three pseudo-spin components vanish identically.

The case of next near neighbor pairs (electrons separated by a primitive lattice vector
in the basal plane) turns out to be identical to the on-site case. This is expected, since a
primitive lattice vector is involved. Formally, the group for two fixed sites separated by a
lattice vector is \( C_s \) composed of the identity, \( E \), and \( \sigma_h \). There are two representations
of this group, \( \Gamma_1 \) (even \( z \)) and \( \Gamma_2 \) (odd \( z \)). The former is only composed of even \( M_J \) pairs, the
latter of odd \( M_J \) pairs. When the full space group is considered (that is, all rotations of the
two sites plus their interchange), then \( \Gamma_1 \) leads to the even \( z \) representations, \( \Gamma_2 \) to the odd
\( z \) representations, and thus the arguments of the above paragraph follow immediately.

The case of near neighbor pairs (electrons separated by a non-primitive lattice vector)
is somewhat different. In this case, one electron is at site 1 in the primitive cell, the other
at site 2. Again using the properties of the single particle wavefunctions discussed above,
for the \( k_z = 0 \) case, only odd (even) \( M_J \) states are non-vanishing for the combination \( k, Pk \)
(\( k, Tk \)) just as before. On the other hand, for the \( k_z = \pi/c \) case, only odd \( M_J \) states
are non-vanishing for both combinations (previously, it was even \( M_J \)). To complete the
argument, though, one needs to know how even $z$ and odd $z$ representations transform. A key difference from before is due to the $c$ axis being a screw axis. Thus, the operation $\sigma_h$ must be followed by a non-primitive translation. In the previous paragraphs, this resulted in a phase factor of unity since the pairs $k, -k$ involved electrons either both at atom site 1 or both at atom site 2 (modulo a primitive lattice vector). In the present case, though, one of the electrons is at site 1, the other at site 2, resulting in an overall phase factor of $e^{ik_zc}$ where $c$ is the lattice constant along the $c$ axis. Thus the effect of $\sigma_h$ on a pair is $(-1)^{M_J}e^{ik_zc}$. For odd (even) $z$ representations, then, $M_J$ must be odd (even) for $k_z = 0$ and even (odd) for $k_z = \pi/c$ to be non-vanishing. Combining this with the constraints of the single particle wavefunctions mentioned earlier, one then finds the same results as before. That is, for odd $z$ representations, $d_x$ and $d_y$ are non-vanishing and $d_z$ vanishing for $k_z = 0$, but for $k_z = \pi/c$, all vanish; whereas for even $z$ representations, $d_x$ and $d_y$ are vanishing and $d_z$ non-vanishing for $k_z = 0$, but all are non-vanishing for $k_z = \pi/c$.

The above arguments have implications, at least for the case of $U Pt_3$. The calculated Fermi surface for $U Pt_3$ has two of the five Fermi surface sheets centered about the $k_z = \pi/c$ zone face (contributing about 43% to the total density of states$^{13}$ and both sheets are in good agreement with deHaas-vanAlphen data$^{14}$. Therefore, the existence of line nodes in $U Pt_3$ cannot be used as a criterion to differentiate between even and odd parity pairing, since given the above arguments, two of the five sheets will have line nodes for three of the possible six odd parity representations, even if the pair state involves all three components of the $d$ vector.

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