Odd parity and line nodes in heavy-fermion superconductors

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(Received 15 June 1995)

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.

The symmetry of the order parameter of heavy-fermion superconductors is still an unresolved issue after over a decade's worth of work.[1] 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.[2,3] In particular, Blount showed that a general odd-parity order parameter would not have line nodes in the presence of spin-orbit coupling.[3] 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 close-packed lattice, such as UPt_3, where it will be shown that three of the six odd-parity representations vanish. The proof is by construction, taking into account the product nature of the pair wave function, under the condition that the pairing is due to the f electrons. This involves analyzing the pair wave function of f electrons separated by primitive and nonprimitive lattice vectors.

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[4] (Blount's argument, though, is general and does not depend on the use of basis functions). For instance, consider the E_{1u} (Γ_5^-) representation. Basis functions at the p-wave level are $k_z(\hat{\mathbf{x}}\pm i\hat{\mathbf{y}})$ and $(k_x\pm ik_y)\hat{\mathbf{z}}$ where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ 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[5] and Sauls[6] where only the $S_z=0$ component is kept). An exception was a recent model of Norman[7] which treated the strong spin-orbit limit of on-site pairing. In this case, it was found that the Γ_6^- (E_{2u}) pair state vanished on the $k_z=\pi/c$ zone face. The question is whether this result is specific to on-site pairing of f electrons 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 wave functions. The f electron part of the single-particle wave functions is a linear combination of $J=5/2$ functions (where J denotes the total angular momentum[8]). In the case of a hexagonal close-packed lattice, there are two f atoms per primitive cell (separated by a nonprimitive translation vector). Therefore, the wave function is of the form $a_{\mu i}^{n\vec{k}}|\mu\rangle_i$ where n is a band index, μ a basis function ($-5/2,-3/2,-1/2,1/2,3/2,5/2$), and i 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 $z\rightarrow -z$ (σ_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.[9] 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_μ 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 $e^{i\vec{k}\cdot\vec{r}}$ will introduce a relative phase between the two sites of 1 for $k_z=0$ and -1 for $k_z=\pi/c$.

Now consider basis functions for pairs of f electrons. Since a center-of-mass momentum of zero is assumed (that is, $\vec{k}$ and $-\vec{k}$ are paired), these pairs are from representations at the Γ point of the zone (Γ_1 through Γ_6). In addition, the correct combination of these pair states corresponding to either even or odd parity must be constructed. This was considered in the presence of spin orbit by Anderson.[10] 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 $-\vec{k}$ can be labeled as Pk and Tk. The even parity combination is then $k,Tk-PTk,Pk$ and is a pseudospin singlet (corresponding to $S=0$ in the spin only case). For odd parity, there are three pseudospin 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 wave function in real space. The cases of electrons on the same site, electrons separated by a nonprimitive lattice vector, and electrons separated by a primitive lattice vector have been treated by Appel and Hertel[9] (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 wave function (assuming the pairing is due to the f electrons) since all f atom sites are connected by either a primitive or nonprimitive lattice vector.

For on-site pairs (the case treated in Ref. 7), three of the six possible odd-parity representations, labeled even z representations (Γ_1^-, Γ_2^-, Γ_5^-), involve states with even M_J, the other three, labeled odd z representations (Γ_3^-, Γ_4^-, Γ_6^-), involve states with odd M_J.[11] 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 μ and $-\mu$). For $k_z=0$, using the relations satisfied by the single-particle wave functions, combinations like k,Pk are nonvanishing only for odd M_J states whereas combinations like k,Tk are nonvanishing only for even M_J states.[12] Thus, for even z representations, d_x and d_y vanish, whereas for odd z representations, d_z vanishes. This is the familiar result which was illustrated by basis functions[4] in the first part of this paper (these 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 wave functions discussed above. In this case, only even M_J states are nonvanishing for both k,Pk and k,Tk combinations. Therefore, for even z representations, all three pseudospin components are, in general, nonzero on this face, whereas for odd z representations, all three pseudospin 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 σ_h. There are two representations of this group, Γ_1 (even z) and Γ_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 Γ_1 leads to the even z representations, Γ_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 nonprimitive 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 wave functions discussed above, for the $k_z=0$ case, only odd (even) M_J states are nonvanishing 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 nonvanishing 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 σ_h must be followed by a nonprimitive 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 σ_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 nonvanishing. Combining this with the constraints of the single-particle wave functions mentioned earlier, one then finds the same results as before. That is, for odd z representations, d_x and d_y are nonvanishing 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 nonvanishing for $k_z=0$, but all are nonvanishing for $k_z=\pi/c$.

The above arguments have implications, at least for the case of UPt_3. The calculated Fermi surface for UPt_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 de Haas–van Alphen data.[14] Therefore, the existence of line nodes in UPt_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.

This work was supported by the U.S. Department of Energy, Basic Energy Sciences, under Contract No. W-31-109-ENG-38. The author also acknowledges the support of the Aspen Center for Physics where this work was begun.

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