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Space-group approach to two-electron states in unconventional superconductors

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The direct application of the space-group representation theory, makes possible to obtain limitations for the symmetry of SOP on lines and planes of symmetry in one-electron Brillouin zone. In the case of highly symmetric UPt_3 only theoretical nodal structure of IR E_{2u} is in agreement with all the experimental results. On the other hand, in the case of high-T_c-superconductors the two electron description of Coper pairs in D_{2h} symmetry is not sufficient to describe experimental nodal structure. It was shown that in this case, the nodal structure is the result of underlying interactions between two-electron states and hidden symmetry D_{4h}.

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1. Introduction

Unconventional superconductivity is connected with different symmetry violations and the superconducting order parameter in these materials vanishes at points and lines on Fermi-surface [1]. Time-reversal symmetry is violated in heavy fermion superconductors $(UTh)Be_{13}$, Sr_2RuO_4, $PrOs_4Sb_{12}$ [2] and high-temperature superconductors [3]. The nodal structure of unconventional superconductors was investigated by virtue of point-group approach [1, 4, 5] and a space-group approach [6-11]. The space-group approach is based on space-group irreducible representations (IRs) for one-electron wave functions [12] and on the assumption of Ginzburg and Landau [13] that superconducting order parameter (SOP) is identical with the wave function of a Cooper pair.

2. Space group approach

The general principles of constructing singlet and triplet pairs were formulated by Anderson [14]. In a spherically symmetric case, the electrons in a Cooper pair have opposite momentums. The wave function of the pair is antisymmetric with respect to permutations and invariant under lattice translations, and transforms according to the IR of the point group. The spatial parts of singlet and triplet pairs a given by two following formulae:

$$\Phi_1^s = \varphi^1\varphi_I^2 + \varphi_I^1\varphi^2 \quad (1),$$

$$\Phi_1^t = \varphi^1\varphi_I^2 - \varphi_I^1\varphi^2 \quad (2)$$

Superscripts denote the number of electronic coordinate and subscript *I* corresponds to the action of space inversion on the initial spatial function. The wave function of a singlet pairs is even, and that of triplet pairs is odd. In real crystals, the wave function of electrons is characterized by the star $\{\boldsymbol{k}\}$ of wave vector $\boldsymbol{k}$. Clearly, a correct translation-invariant two-electron function must be antisymmetric with respect to permutations and must be a linear combination of the functions belonging to all the prongs of the star $\{\boldsymbol{k}\}$. The structure of such a function depends on vector $\boldsymbol{k}$ and its symmetry group H. On the directions and planes of symmetry one-electron wave functions φ are transformed according to IR *D* of group *H* and thus the symmetry of two-electron functions (1) and (2) is more complex. It follows from the induced representation theory [12], that the symmetry properties of function (1) and (2) on directions and planes of symmetry are defined by their characters on the group *M=H+IH*:

$$\chi^{\pm}(h) = \chi^2(D(h)) \quad (3)$$

$$\chi^{\pm}(Ih) = \pm\chi(D(IhIh)) \quad (4),$$

where plus sign corresponds to the singlet pair, minus sign corresponds to the triplet pair and *h* is an element of group *H*. To obtain the total basis set one should act on these functions by the pure rotational elements transforming the initial $\boldsymbol{k}$-vector into other prongs of its star and to decompose it into irreducible basis sets. This procedure is simplified by the Frobenius reciprocity theorem [6-12], according to which only those IRs of the whole group *G* are possible, whose characters are not orthogonal to characters (3), (4). The analysis for the planes of symmetry is given in Table 1. The relevant subgroup C_{2h} has two even and two odd IRs. The singlet transforms according to IR A_g of C_{2h} subgroup. The absence of the other IR B_g means that some even IRs of he group *G* are forbidden at the plane of symmetry. If one of such IRs corresponds to Cooper pairing, the SOP of this symmetry

has nodes on this plane. The intersection of this plane with Fermi-surface results in line of nodes. The spatial part of triplet function also has line nodes, but when this function is multiplied by triplet spun function, transforming according to IR T_{2g} in O_h group, total wave function contains all IRs of C_{2h} group. This case corresponds to the Blount theorem [5]. In axial symmetry groups, like D_6h, spin parts M_s=+1 and M_s=-1 (ferromagnetic spin orientation, IR E_{1g}) transform independently from pair with M_s=0 (antiferromagnetic spin orientation, IR A_{2g}) and lines of nodes are required by the symmetry.

Table 1. Nodal structure of two-electron states on the planes of symmetry for groups O_h and D_{6h}.

G	Type of character	Symmetry element				IR of C_{2h}	Structure on the w.f.
		E	σ_h	I	C_2		
O_h, D_{6h}	χ^+	1	1	1	1	A_g	nodes
O_h, D_{6h}	χ^-	1	1	-1	-1	B_u	nodes
O_h	$\chi^-\times\chi(T_{1g})$	3	-1	-3	1	$2A_u+B_u$	no nodes
D_{6h}	$\chi^-\times\chi(E_{2g})$	2	-2	-2	2	$2A_u$	nodes
D_{6h}	$\chi^-\times\chi(A_{2g})$	1	1	-1	-1	B_u	nodes

Let us consider as an example of the odd [15] and antiferromagnetic [16] superconductor UPt_3 (D_{6h} symmetry). Making use of the last line of Table 1 and Frobenius reciprocity theorem possible IRs for antiferromagnetic odd pairs are listed in Table 2.

Table 2. Possible IRs for triplet antiferromagnetic Cooper pairs in D_{6h}. symmetry.

Planes of symmetry	НП D_{6h}
σ_h	$B_{1u}+B_{2u}+E_{1u}$
σ_v	A_{1u}, B_{1u}, E_{1u}, E_{2u}
σ_v'	A_{1u}, B_{2u}, E_{1u}, E_{2u}
Direction Z[1)]	A_{1u}

1) For one-dimensional IRs of H.

If the wave vector of an electron is parallel to the Z axis, the wave vector group H is C_{6v} and the symmetry group M of the pair is D_{6h}. In this case the result depends on the symmetry of one-electron function φ with respect of rotations around the axis. We consider here the one-dimensional small IR for which the symmetry of spatial part of two-electron function is A_{2u}.

Experimental data [17] indicate that there is a line of zeros in the basal plane. It follows from the Table 2, that the corresponding IRs are A_{1u}, A_{2u}, and E_{2u}, which are not among the possible IRs for antiferromagnetic triplet pairs. There is also experimental evidence [17] that the SOP becomes zero at a point on the vertical axis. In light of this, the A_{2u} IR, which has lines of zeros in vertical planes, and theA_{1u} IR, which does not have zero in the vertical direction, must be discarded. The remaining IR, E_{2u}, has zero at a point in the vertical direction and in basal plane. Thus, the nodal structure of the SOP of E_{2u} symmetry for an antiferromagnetic phase of D_{6h} symmetry agrees with all experimental data on the symmetry of the SOP of UPt_3. This conclusion is in line with simulation results [18]. Magnetization anisotropy data for UPt_3 in the superconducting state can only be accounted for by the E_{1g} and E_{2u} IRs [19]. Given that the SOP is odd, this also gives the IR E_{2u}.

Table 3. Spatial parts of Cooper pair wave functions for point groups D_{2h} and D_{4h} and their nodal planes.

D_{2h}			D_{4h}		
IR	Pairing function	nodes	IR	Pairing function	nodes
A_g	$\Phi^s+\Phi^s_{C2x}+\Phi^s_{C2y}+\Phi^s_{C2z}$	no	A_{1g}	$\Phi^s+\Phi^s_{C2x}+\Phi^s_{C2y}+\Phi^s_{C2z}+\Phi^s_{C2d'}+\Phi^s_{C4}+\Phi^s_{C4}+\Phi^s_{C2d}$	no
B_{1g}	$\Phi^s-\Phi^s_{C2x}-\Phi^s_{C2y}+\Phi^s_{C2z}$	σ_x, σ_y	A_{2g}	$\Phi^s-\Phi^s_{C2x}-\Phi^s_{C2y}+\Phi^s_{C2z}-\Phi^s_{C2d'}+\Phi^s_{C4}+\Phi^s_{C4}-\Phi^s_{C2d}$	σ_x, σ_y, σ_{xy}, σ_{-xy}
B_{2g}	$\Phi^s-\Phi^s_{C2x}+\Phi^s_{C2y}-\Phi^s_{C2z}$	σ_z σ_x	B_{1g}	$\Phi^s+\Phi^s_{C2x}+\Phi^s_{C2y}+\Phi^s_{C2z}-\Phi^s_{C2d'}-\Phi^s_{C4}-\Phi^s_{C4}-\Phi^s_{C2d}$	σ_{xy}, σ_{-xy}
B_{3g}	$\Phi^s+\Phi^s_{C2x}-\Phi^s_{C2y}-\Phi^s_{C2z}$	σ_z, σ_y	B_{2g}	$\Phi^s-\Phi^s_{C2x}-\Phi^s_{C2y}+\Phi^s_{C2z}+\Phi^s_{C2d'}-\Phi^s_{C4}-\Phi^s_{C4}+\Phi^s_{C2d}$	σ_x, σ_y,
A_u	$\Phi^t+\Phi^t_{C2x}+\Phi^t_{C2y}+\Phi^t_{C2z}$	σ_x, σ_y, σ_z	E_g^α	$\Phi^s+\Phi^s_{C2x}-\Phi^s_{C2y}-\Phi^s_{C2z}$	σ_y, σ_z
B_u	$\Phi^t-\Phi^t_{C2x}-\Phi^t_{C2y}+\Phi^t_{C2z}$	σ_z		$\Phi^s_{C2d'}-\Phi^s_{C4}+\Phi^s_{C4}-\Phi^s_{C2d}$	σ_y, σ_z
B_{2u}	$\Phi^t-\Phi^t_{C2x}+\Phi^t_{C2y}-\Phi^t_{C2z}$	σ_y	E_g^β	$\Phi^s_{C2d'}+\Phi^s_{C4}-\Phi^s_{C4}-\Phi^s_{C2d}$	σ_x, σ_z
B_{3u}	$\Phi^t+\Phi^t_{C2x}-\Phi^t_{C2y}-\Phi^t_{C2z}$	σ_x		$\Phi^s-\Phi^s_{C2x}+\Phi^s_{C2y}-\Phi^s_{C2z}$	σ_x, σ_z

When acting by projection operators on functions (1) and (2), we obtain the total two-electron functions with zero total momentum for groups D_{2h} and D_{4h}, listed in Table 3. It follows from the induced representation theory, that the multiplicity of the appearance of each IR is equal to its dimensionality. Since the 2D IRs of group D_{4h}

appear twice, additional quantum numbers are needed to classify them. Projecting the initial basis function onto the first line, we obtain the basis designated as E_g^{α} . Starting projection from the second line, we obtain the basis designated as E_g^{β}.

At a general point in the Brillouin zone, all even IRs are possible for singlet pairs, and all odd IRs, for triplet pairs. It follows from formulae (3) and (4) that in the symmetry planes of the Brillouin zone, however, some linear combinations may become zero. Approaching a symmetry plane σ_h in the Brillouin zone, *k*- vector approaches its mirror reflection $\sigma_h \boldsymbol{k}$, and the basis functions Φ^s approach their mirror reflections $\sigma_h\Phi^s$ Two cases are possible in a symmetry plane σ_h. If the basis wave functions Φ^s and $\sigma_h \Phi^s$ appear in a linear combination with opposite signs, this combination becomes zero in the symmetry plane. An intersection of such a plane with the Fermi surface gives a line of zeros of the wave function. If the basis wave functions Φ^s and $\sigma_h \Phi^s$ appear in such a linear combination with the same sign, there are no symmetry grounds for the function to become zero. Since mirror reflection in a plane is equal to the product of a 180^o rotation about the normal to the plane with inversion, and inversion has already been used in constructing the basis functions, to investigate the nodal structure of functions it is sufficient to examine their behavior with respect to rotations only. The function of a singlet (triplet) pair is zero in a plane if, under the action of a 180^o rotation about the normal to the plane the function changes sign (does not change sign), The results of such a study of wave functions of pairs are presented in Tables 3 The results for 1D representations are unambiguous. Since 2D IRs in group D_{4h} appear twice, the results of symmetry analysis for them are somewhat ambiguous. This conclusion is in line with the results reported by Volovik and Gor'kov [4], who obtained two types of basis functions for 2D IRs and three types for 3D IRs. The results obtained in the weak spin-orbit coupling approximation are also valid for singlet pairs in the case of strong spin-orbit coupling. To construct the triplet basis functions one should include the spin function in projecting.

Angle-resolved photoelectron spectra [20] and conductivity spectra [21] indicate that the pseudogap in high-T_c-superconductors is anisotropic and is zero on the diagonals of a rectangle. Analysis of experimental data has led most researchers [22] to conclude that the SOP in high-T_c-superconductors belongs to the A_g IR of group D_{2h}. In connection with this, two possibilities are considered: *s*-pairing, i.e., with no line of zeros, and *d*- pairing, with a line of zeros on the diagonals of a rectangle. In some cases, these pairing types were found to interact [22].

It follows from the data in Table 3 that, in the case of singlet pairs, corresponding to high-T_c-superconductors, all of the IRs except A_g have lines of zeros in the coordinate planes, which cannot be observed experimentally. Moreover, none of the IRs have zeros in the diagonal planes. It follows from the former observation that A_g pairing is the most likely. The second conclusion is trivial since reflection in the diagonal planes is not a symmetry element of group D_{2h}. Thus, the observed nodal structure of electron pairs is more sophisticated than the structure stemming from the crystal symmetry.

To describe the symmetry of such a wave function, let us choose two vectors, $\boldsymbol{k}_{\alpha}$ and $\boldsymbol{k}_{\beta}$, symmetric with respect to the diagonal of the rectangle. The singlet wave functions Φ^s_{α} and Φ^s_{β}, corresponding to the IR A_g can be obtained from Table 3 by introducing additional subscripts α and β. Note that the two-electron states corresponding to different one-electron vectors $\boldsymbol{k}$ belong to the same IR, A_g in the space of two-electron states, and, in contrast to one-electron states belonging to different $\boldsymbol{k}$, may interact. The two resulting states can be written in the form

$$\Phi^s_s = c_1(\Phi^s + \Phi^s_{C2x} + \Phi^s_{C2y} + \Phi^s_{C2z}) + c_2(\Phi^s_{C2d'} + \Phi^s_{C4} + \Phi^s_{C4^{-}} + \Phi^s_{C2d}) \quad (5)$$

$$\Phi^s_{x2-y2} = c_2(\Phi^s + \Phi^s_{C2x} + \Phi^s_{C2y} + \Phi^s_{C2z}) + c_1(\Phi^s_{C2d'} + \Phi^s_{C4} + \Phi^s_{C4^{-}} + \Phi^s_{C2d}) \quad (6)$$

The former function is nonzero in the diagonal planes and is labeled with subscript s; the latter function approaches zero in the diagonal planes and is labeled with subscript $x^2 - y^2$. Note that the degree of orthorhombicity, quantified by (b-a)/(b + a), in YBaCuO materials is as low as about 2% [22] and can be thought of as perturbation. In the symmetry group D_{4h}, function (5) belongs to the IR A_{1g} , and function (6) belongs to the IR B_{1g} The latter function is zero on the diagonals, in agreement with experiment [20-22]. Thus, it follows from the present group-theoretical analysis, that the two-electron wave function in the high-T_c-superconductors corresponds to the IR B_{1g} of group D_{4h} rather than to the IR A_{1g} of group D_{2h}.

3. Conclusions

In a conclusion, the direct application of the space-group representation theory, makes possible to obtain limitations for the symmetry of SOP on lines and planes of symmetry in one-electron Brillouin zone. In the case of highly symmetric UPt_3 only theoretical nodal structure of IR E_{2u} is in agreement with all the experimental results. On the other hand, in the case of high-T_c-superconductors the two electron description of Coper pairs in D_{2h} symmetry is not sufficient to describe experimental nodal structure. It was shown that in this case, the nodal structure is the result of underlying interactions between two-electron states and hidden symmetry D_{4h}.

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