Space-group approach to the wavefunction of a Cooper pair and its application to hight-T_c superconductors

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Abstract

The general two-electron wavefunctions obeying the Pauli exclusion principle and Anderson criteria for Cooper pairs are constructed for D_{2h} and D_{4h} symmetries. It is shown that in axial symmetry groups the Blount theorem is violated and lines of nodes of triplet superconducting order parameter are required by the symmetry..Application of the results to hight-T_c superconductors and feroomagnetic sureconductor UPt_3 are discussed.

1 Introduction

The signature of unconventional superconductivity, both heavy fermion (HF) and high -T_c, is a breaking of di¤erent symmetries, including time reversal symmetry. In contrast with standard BCS superconductivity where superconducting order parameter (SOP) is totally symmetric (belongs to a_{1g} irreducible representation (IR)), SOP of unconventional superconductors belongs to others IRs of point groups. We refer the reader to two reviews on high -T_c [1] and HF [2] superconductors. Since the underlying symmetries of unconventional superconductors are very signi…cant in understanding of their pairing nature, there are three di¤erent group theoretical approaches to the description of the SOP symmetry: point group approach [2, 3, 4, 5, 6, 7, 8, 11, 12, 13, 14] , space-group approach [15, 16, 18, 19, 20, 21] and unitary group approach.[22, 23, 24]. The SOP symmetry of high -T_c superconductors was considered in a framework of all these approaches [11, 12, 13, 14, 19, 22, 23]

The starting point of all approaches is the Anderson [3] description of the Cooper pair in ($\vec{k}$-$\vec{k}$) manifold.

Anderson showed that the wavefunctions of electrons in a singlet pair are connected by the time-reversal and the pairing operator is written as:

$$\left\langle C^{+}_{k} C^{+}_{-k} \right\rangle \left\langle C^{+}_{-k} C^{+}_{k} \right\rangle \left\langle C^{+}_{\uparrow} C^{+}_{\downarrow} - C^{+}_{\downarrow} C^{+}_{\uparrow} \right\rangle \quad (1)$$

The wavefunctions of electrons in a triplet pair are connected by the time-reversal, space inversion and their product The three components of the wavefunction for a triplet case, corresponding to $M_s = 1, 0, -1$ are written as:

$$\left\langle C^{+}_{k} C^{+}_{-k} \right\rangle - \left\langle C^{+}_{-k} C^{+}_{k} \right\rangle \left\langle C^{+}_{\uparrow} C^{+}_{\uparrow} \right\rangle \quad (2)$$

$$\mathbf{D} \qquad \mathbf{ED} \qquad \mathbf{E}$$
$$C^{\dagger}_{k}C^{\dagger}_{-k} - C^{\dagger}_{-k}C^{\dagger}_{k} \quad C^{\dagger}_{\uparrow}C^{\dagger}_{\#} + C^{\dagger}_{\#}C^{\dagger}_{\uparrow} \tag{3}$$

$$\mathbf{D} \qquad \mathbf{ED} \qquad \mathbf{E}$$
$$C^{\dagger}_{k}C^{\dagger}_{-k} - C^{\dagger}_{-k}C^{\dagger}_{k} \quad C^{\dagger}_{\#}C^{\dagger}_{\#} \tag{4}$$

The Cooper pair's wavefunction is invariant with respect to lattice translations, hence it belongs to irreducible representation of point group and is characterized by parity [3].

In a point group approach the symmetry of the SOP is described in terms of algebraic functions belonging to the IRs of point group under consideration and hence its conclusions depend on the choice of basis functions and are ambiguous [10]. The results of point group approach in many cases correctly re‡ect symmetry properties of SOP, but they can't be used in quantum mechanical calculations, since they do not express Cooper pair wavefunction as two-electron wavefunction obeying the Pauli exclusion principle. The power-low temperature dependence of physical properties below T_c indicates that the superconducting gap vanishes at points and on the lines at Fermi surface [1, 2]. According to the Blount theorem, there are no group-theoretical requirement for the triplet SOP in a strong spin- orbit coupling case [5].

The basic idea of a space group approach is to construct general two electron wavefunction on the basis of the correct functions belonging to the space-group IRs and retain only those pairs for which the Anderson criteria are ful…lled. The space group approach was used to …nd all possible IR for Cooper pair wavefunction but the general wavefunction of Cooper pairs were not constructed so far. It was also shown that di¤erent types of time-reversal symmetry violations result in violations of the Blount theorem [19, 20, 21].

In the present work the induced representation method is applied to obtain the nodal structure of SOP for D_{2h} and D_{4h} symmetries. It is also shown that the violations of the Blount theorem may be connected with symmetry breaking from highest point symmetry O_h to axial point group symmetry. General two-electron wavefunction are constructed for D_{2h} and D_{4h} symmetries making use of Anderson formulae (1), (2), (3), (4). and standard projection operators technique. Applications of the theoretical results to high -T_c superconductors and HF superconductor UPt_3 are discussed.

2 Theory

2.1 Induced representation method

The one-electron states in a solid are labelled by two quantum numbers: the wave vector $\vec{k}$ taken in the representation domain of a Brillouin zone and the index κ of small IR q_κ of the wave vector group H [25, 26, 27, 28] . The structure of IR of the space group G depends on the left coset decomposition of G with respect to H:

$$G = \sum_{i} s_i H, \; i = 1 \ldots |G| / |H| \tag{5}$$

Where jj stands for the number of elements in a group. The action of rotational elements of coset representatives s_i results in all prongs of the wave vector star $\{\vec{k}\}$.

The induced representation is de…ned by the following formula:

$$(q_\kappa \uparrow G)(g)_{i\mu,j\nu} = q_\kappa(s_i^{-1} g s_j)_{\mu\nu} \delta(s_i^{-1} g s_j, H) \tag{6}$$

where: $\delta(s_i^{-1} g s_j, H) = \begin{cases} 1, \; if \; s_i^{-1} g s_j \in H \\ 0, \; if s_i^{-1} g s_j \notin H \end{cases}$

If the basis set of IR q_κ fϕ_kg is known , the basis set of induced representation is obtained by the action left coset representatives on it :

$$\text{f©g} = \sum_i s_i \text{f}\phi_k\text{g}, \; i = 1 \ldots \text{j}G\text{j} / \text{j}H\text{j} \tag{7}$$

The induced representation and its basis set de…ned by formula (7) may be or. may not be irreducible. In the case of the space group G and its little group H the induced representation (6) is irreducible and is used throughout [25, 26, 27, 28] in solid state physics.

Since the symmetry of one-electron states is de…ned, they will be used for constructing two-electron states, namely Cooper pair, making used of general principles of quantum mechanics. According to the Pauli exclusion principle the spatial part of a singlet Cooper pair wavefunction belongs to the symmetrized Kronecker square of the IR q_κ " G and the spatial part of a triplet pair belongs to antisymmetrized Kronecker square of the same IR . In the case of strong spin-orbit coupling Cooper pair wavefunction pair belongs to the antisymmetrized Kronecker square of the double-valued IR .

The Kronecker product of induced representation may be decomposed making use of the Mackey theorem on symmetrized squares [26]. Its structure depends on the double coset decomposition of the space group G with respect to the wave vector group H:

$$G = \sum_\sigma H d_\sigma H \tag{8}$$

For every d_σ including identity element we consider an intersection subgroup $M_\sigma = H \setminus d_\sigma H d_\sigma^{-1}$ and its representation de…ned by the formula:

$$P_\sigma = q_\kappa(m) \pounds q_\kappa(d_\sigma^{-1} m d_\sigma) \tag{9}$$

where £ denotes direct (Kronecker) product of representations.

Corresponding wave vector $\vec{k}_\sigma$ is de…ned by the following formula

$$\vec{k} + d_\sigma \vec{k} = \vec{k}_\sigma + \vec{b}_\sigma \tag{10}$$

where $\vec{b}_\sigma$ is a vector of reciprocal lattice.

For $\vec{k}$ a general point in Brillouin zone $\vec{k}_\sigma$equals zero if d_σ is a space inversion. This case corresponds to formulae (1), (2), (3), (4).

For any self-inverse double coset $\sigma = \alpha$ (that is $Hd_\sigma H = Hd_\sigma^{-1}H$) there are two extensions $P_\alpha^\S$ of P_α into extended intersection subgroup $\mathcal{M}_\alpha$:

$$\mathcal{M}_\alpha = M_\alpha + aM_\alpha \tag{11}$$

(where $a = d_\sigma h_1 = h_2 d_\sigma$ and $h_1, h_2 \in H$). These two extensions correspond to symmetrized and antisymmetrized squares. Their characters on group M_α are the same and for the elements of the left coset aM_α are de…ned by two following formulae respectively:

$$\chi(P_\alpha^+(am)) = +\chi(q_\kappa(amam)) \tag{12}$$

$$\chi(P_\alpha^-(am)) = -\chi(q_\kappa(amam)) \tag{13}$$

In the above notations symmetrized and antisymmetrized parts of the Kronecker square of induced representation are written as :

$$[q_\kappa \,"\, G \pounds\, q_\kappa \,"\, G] = [q_\kappa \pounds\, q_\kappa] \,"\, G + \sum_\alpha P_\alpha^+ \,"\, G + \sum_\beta P_\beta \,"\, G \qquad (14)$$

$$\mathsf{f}q_\kappa \,"\, G \pounds\, q_\kappa \,"\, G\mathsf{g} = \mathsf{f}q_\kappa \pounds\, q_\kappa\mathsf{g} \,"\, G + \sum_\alpha P_\alpha^{¡} \,"\, G + \sum_\beta P_\beta \,"\, G \qquad (15)$$

The …rst items on the right correspond to the double coset de…ned by the identity element for which the small representations q_κ are symmetrized (antisymmetrized) over the H group. The sums in the second items correspond to the self-inverse double cosets discussed above and the third items correspond to the not self-inverse double cosets for which $Hd_\beta H \neq Hd_\beta^{¡1}H$. It follows from the Mackey theorem that types of quasi-particles which it is possible to construct from two equivalent electrons depend on the double coset decomposition of the space-group with respect to the wave vector group. Hence these types depend on the position of a wave vector in one-electron Brillouin zone. In the present work we consider pairs corresponding to the double coset de…ned by the space inversion. It follows from formula (10) that the wave vector of a Cooper pair equals zero in this case and its wavefunctions are classi…ed according to IRs of the point group $\hat{G}$ which is a central extension of a space group G.

For $\vec{k}$ a general point in a Brillouin zone the extended intersection subgroup $\mathcal{M}_\alpha$ is a group C_i consisting of the identity element E and the space inversion I. It follows from formulae (9), (12) and (13) that the spatial part of a singlet pair belongs to IR A_g and the spatial part of a triplet pair belongs to IR A_u of a group C_i. The induced representations $P_\alpha^{\S} \,"\, G$ may be decomposed making use of Frobenius reciprocity theorem [28].: the number of appearance of the IR ¡ of the group G in the decomposition of the induced representation $P_\alpha^{\S} \,"\, G$ equals to the number of appearance of the IR $P_\alpha^{\S}$ in the decomposition of ¡ when it subduced to H. Hence for $\vec{k}$ a general point in a Brillouin zone we obtain that for the spatial part of a singlet pair all even representations are possible and for the spatial part of a triplet pair all odd representations are possible. The same conclusion is also valid for total wavefunctions of Copper pairs since multiplication by even spin singlet S^0 and spin triplet S^1 wavefunctions doesn't change parity. It also follows from Frobenius reciprocity theorem that for $\vec{k}$ a general point in a Brillouin zone the number of appearance of any IR (even for singlet pairs and odd for triplet pairs) equals to its dimension. As the result, for two-dimensional IRs (E_g and E_u in D_{4h} symmetry) two linearly independent basis sets are possible. This is illustrated in the next section by direct construction of the basis set.

We adopt Kovalev's [25] notations for the point group operations, which are presented in Appendix.

On the planes of symmetry in Brillouin zone the little group H contains a re‡ection operators and the extended intersection group $\mathcal{M}_\alpha$ consists of four elements.

The characters of symmetrized and antisymmetrized Kronecker squares belong to IRs A_g and A_u respectively. Since not all the IRs of the group C_{2h} are present, it follows from the Frobenius reciprocity theorem, that some of the IRs of the whole group are forbidden if the $\vec{k}$ vector is on this plane. The intersection of this plane with the Fermi surface results in a line of nodes of any particular IR. If ,for example, this IR is responsible for superconductivity this corresponds to the line of nodes of superconducting order parameter. In a weak spin-orbit coupling case lines of nodes follows from the symmetry both for triplet and singlet pairs.

In a strong spin-orbit coupling case spins of electrons are coupled with their spatial parts in each $\vec{k}$ ¡ $\vec{k}$ manifold. To obtain the characters of the total wavefunction one should multiply the characters of the spatial part by the spin singlet and spin triplet wavefunctions..In the highest point symmetry O_h these spin parts belong to IRs A_{1g} and T_{1g} respectively. The character for the singlet pair is unchanged, but the decomposition of the character in a triplet case contains

characters of all IRs of group C_{2h}. This means that there are not symmetry requirements for the lines of nodes for triplet pairs in a strong spin-orbital case. (Blount theorem [5]). When the symmetry is reduced from the highest point symmetry O_h to axial symmetry group D_{4h} the IR of spin triplet wavefunction is reduced to two A_{2g} and E_g. Decomposition $P_\alpha^{\dagger}$ £ E_g # C_{2h} contains two IRs $2A_u$ of group C_{2h} and it follows that not all odd IR appear in the induced representation. Similar consideration is valid for the product $P_\alpha^{\dagger}$ £ A_{2g} # C_{2h}. If the interaction of electron spin with lattice is not negligible the spin states E_g and A_{2g} are splitted and generally speaking only one of them corresponds to Cooper pairs. Hence it follows that lines of nodes are possible for triplet states in strong spin-orbit coupling case. Similar decomposition is presented in Table 1. for all planes of symmetry of group D_{2h}. For all planes the spin is of pair is directed in z direction. This approach corresponds to strong interaction of electron spin with lattice. Note that in Refs. [19, 20, 21] spin-lattice interactions were neglected and spin was quantized along the directions perpendicular to the planes.

Table 1. Decomposition of Kronecker products for different planes of symmetry

product	character				decomposition
	E	σ_h	I	C_2	
P_α^{+}	1	1	1	1	A_g
$P_\alpha^{\dagger}$	1	1	¡ 1	¡ 1	B_u
plane (001)	h_1	h_{28}	h_{25}	h_4	
$P_\alpha^{\dagger}$ £ E_g # T_{1g}	3	¡ 1	¡ 3	1	$2A_u$ + B_u
$P_\alpha^{\dagger}$ £ E_g # C_{2h}	2	¡ 2	¡ 2	2	$2A_u$
$P_\alpha^{\dagger}$ £ A_{2g} # C_{2h}	1	1	¡ 1	¡ 1	B_u
plane (100)	h_1	h_{26}	h_{25}	h_2	
$P_\alpha^{\dagger}$ £ E_g # C_{2h}	2	0	¡ 2	0	A_u + B_u
$P_\alpha^{\dagger}$ £ A_{2g} # C_{2h}	1	¡ 1	¡ 1	1	A_u
plane (110)	h_1	h_{40}	h_{25}	h_{16}	
$P_\alpha^{\dagger}$ £ E_g # C_{2h}	2	0	¡ 2	0	A_u + B_u
$P_\alpha^{\dagger}$ £ A_{2g} # C_{2h}	1	¡ 1	¡ 1	1	A_u

Making use of Table 1 and Frobenius reciprocity theorem possible IRs of Cooper pairs are constructed for groups D_{2h} and D_{4h} and presented in Tables 2 and 3. If IR responsible for the Cooper pairing is known, the absence of this IR in the decomposition for any plane indicated line of nodes of SOP. On the other hand if experimental nodal structure of SOP is known comparison with theoretical data may be useful to obtain index of IR responsible for Cooper pairing.

Table 2. Possible IRs of spatial parts of Cooper pairs for $\vec{k}$ at the planes of symmetry. D_{2h} point group.

plane(001)	
weak S-O coupling	
singlet	A_g + B_{1g}
triplet	B_{2u} + B_{3u}
strong S-O coupling	
triplet ($\hat{x}$,$\hat{y}$)	$2A_u$ + $2B_{1u}$
triplet ($\hat{z}$)	B_{2u} + B_{3u}
planes (100) and (010)	
weak S-O coupling	
singlet	A_g + B_{3g}
triplet	B_{1u} + B_{2u}
strong S-O coupling	
triplet ($\hat{x}$,$\hat{y}$)	A_u + B_{1u} + B_{2u} + B_{3u}
triplet ($\hat{z}$)	A_u + B_{3u}

Table 3. Possible IRs of spatial parts of Cooper pairs for $\vec{k}$ at the planes of symmetry. D_{4h} point group.

plane (001)	
weak S-O coupling	
singlet	A_{1g} + A_{2g} + B_{1g} + B_{2g}
triplet	$2E_u$
strong S-O coupling	
triplet ($\hat{x}$,$\hat{y}$)	$2(A_{1u}$ + A_{2u} + B_{1u} + $B_{2u})$
triplet ($\hat{z}$)	$2E_u$
planes (100) and (010)	
weak S-O coupling	
singlet	A_{1g} + B_{1g} + E_g
triplet	A_{2u} + B_{2u} + E_u
strong S-O coupling	
triplet ($\hat{x}$,$\hat{y}$)	A_{1u} + A_{2u} + B_{1u} + B_{2u} + E_u
triplet ($\hat{z}$)	A_{1u} + B_{1u} + E_u
planes (110) and ($\bar{1}$10)	
weak S-O coupling	
singlet	A_{1g} + B_{2g} + E_g
triplet	A_{2u} + B_{1u} + E_u
strong S-O coupling	
triplet ($\hat{x}$,$\hat{y}$)	A_{1u} + A_{2u} + B_{1u} + B_{2u} + E_u
triplet ($\hat{z}$)	A_{1u} + B_{2u} + E_u

2.2 Projection operator technique

For for $\vec{k}$ a general point in a Brillouin zone the basis function belonging to the group $\mathbb{M}_\alpha$ are the Anderson functions for singlet and triplet cases. The basis functions for the whole group may be obtained by projection operators technique. Let us denote $\vec{k}_1$ the wave vector chosen in the representation domain of a Brillouin zone. Making use of Kovalev's notation h_{25} for the space inversion the spatial parts of Anderson singlet and triplet functions are written as:

$$©_1^s = \psi_1^1\psi_{25}^2 + \psi_{25}^1\psi_1^2 \tag{16}$$

$$©_1^t = \psi_1^1\psi_{25}^2 - \psi_{25}^1\psi_1^2 \quad (17)$$

Where the superscript of ψ denotes the number of electronic coordinate and subscript of ψ the prong of the $\vec{k}$-vector star . Subscript of © is the same as that of the …rst appearing ψ_i in the right hand side. The other subscript in right hand side in all cases corresponds to the action of h_{25} on the …rst ψ_i.

Acting by pure rotations belonging to D_{2h} group on these function we can easily obtain all other basis functions:

$$©_2^s = \psi_2^1\psi_{26}^2 + \psi_{26}^1\psi_1^2 \quad (18)$$

$$©_2^t = \psi_2^1\psi_{26}^2 - \psi_{26}^1\psi_2^2 \quad (19)$$

$$©_3^s = \psi_3^1\psi_{27}^2 + \psi_{27}^1\psi_3^2 \quad (20)$$

$$©_3^t = \psi_3^1\psi_{27}^2 - \psi_{27}^1\psi_3^2 \quad (21)$$

$$©_4^s = \psi_4^1\psi_{28}^2 + \psi_{28}^1\psi_4^2 \quad (22)$$

$$©_4^t = \psi_4^1\psi_{28}^2 - \psi_{28}^1\psi_8^2 \quad (23)$$

These functions span the space of Anderson function under the action of all point group operations. Since the space inversion is already included in the basis function, their total number equals to the half of number of point group operations. When action by pure rotations on the initial vector $\vec{k}_1$ result in a star whose number of prongs is half of the number of prongs in the star of wave vector and we call it a halfstar. We assume that the action of the space inversion on the basis vector corresponding to any prong of a halfstar doesn't change a vector but introduces multiplies ¡1 for the triplet case. Making use of standard projection operator technique and functions $©_{1\,i\,4}^{s,t}$ we easily obtain the basis functions for Cooper pairs belonging to all IRs of D_{2h} group. The results are presented in Table 4.

Table 4 Possible spatial parts of singlet Cooper pair wavefunctions in D_{2h} symmetry.

To obtain wavefunctions of triplet pairs one should replace subscripts g to u in the …rst column and all superscripts s to t in the second column without changing of the signs.

IR	wavefunction
A_{1g}	$©_1^s + ©_2^s + ©_3^s + ©_4^s$
B_{1g}	$©_1^s - ©_2^s - ©_3^s + ©_4^s$
B_{2g}	$©_1^s - ©_2^s + ©_3^s - ©_4^s$
B_{3g}	$©_1^s + ©_2^s - ©_3^s - ©_4^s$

Before going to the projection for D_{4h} group is useful to remind that the correspondence of IRs in the subduction $D_{4h} \# D_{2h}$ is as follows: A_1 and B_1 ¡ ! A_1:, A_2 and B_2 ¡ ! B_1, E ¡ ! $B_2 + B_3$. The basis functions for one-dimensional IRs of D_{4h} group are immediately obtained by projection operator technique. Since each of IRs $E_{g(u)}$ appear twice in the Kronecker product decomposition there are two independent basis sets labeled by additional quantum numbers . Bearing in mind the above reduction scheme of IRs we begin with basis sets corresponding to IRs B_2 and B_3 and make use of formula (7). choosing h_{13} as left coset representative we obtain the remainder results of Table 5.

Table 5 Possible spatial parts of singlet Cooper pair wavefunctions in D_{4h} symmetry.

To obtain wavefunctions of triplet pairs one should replace subscripts g to u in the …rst column and all superscripts s to t in the second column without changing of the signs.

IR	pairing function
A_{1g}	$©^s_1 + ©^s_2 + ©^s_3 + ©^s_4 + ©^s_{13} + ©^s_{14} + ©^s_{15} + ©^s_{16}$
A_{2g}	$©^s_1 ¡ ©^s_2 ¡ ©^s_3 + ©^s_4 ¡ ©^s_{13} + ©^s_{14} + ©^s_{15} ¡ ©^s_{16}$
B_{1g}	$©^s_1 + ©^s_2 + ©^s_3 + ©^s_4 ¡ ©^s_{13} ¡ ©^s_{14} ¡ ©^s_{15} ¡ ©^s_{16}$
B_{2g}	$©^s_1 ¡ ©^s_2 ¡ ©^s_3 + ©^s_4 + ©^s_{13} ¡ ©^s_{14} ¡ ©^s_{15} + ©^s_{16}$
$E_g(B_{2g})$	$©^s_{13} ¡ ©^s_{15} + ©^s_{14} ¡ ©^s_{16}$
	$©^s_1 ¡ ©^s_2 + ©^s_3 ¡ ©^s_4$
$E_g(B_{3g})$	$©^s_1 + ©^s_2 ¡ ©^s_3 ¡ ©^s_4$
	$©^s_{13} + ©^s_{15} ¡ ©^s_{14} ¡ ©^s_{16}$

For $\vec{k}$ a general point in a Brillouin zone all IRs are possible for Cooper pair. But when the $\vec{k}$-vector approaches any mirror plane the mirror re‡ection image of $\vec{k}$ also approaches the $\vec{k}$-vector. Total number of states decreases and lines of nodes are eventual. There are two possibilities If two-electron function is unchanged under the action of the re‡ection, the function under consideration is nonvanishing on the mirror plane. On the other hand if the function changes its sign, two mirror counterparts are cancelling on the plane. This corresponds to the line of nodes.

Making use of the above rules and the date of Table A2 we can easily obtain nodal structure of basis functions of one dimensional IRs of groups D_{2h} and D_{4h} presented in Tables 4 and 5. The results are in agreement with the data of tables 2 and 3. obtained making use of Mackey theorem. Two dimensional IRs appear twice for $\vec{k}$ a general point in a Brillouin zone. It is seen from Table 3 that at basal plane two-dimensional IR are forbidden and on vertical planes they appear only once. In this case a direct analysis of nodal structure of basis functions of Table 5 is required. The analysis shows that basis functions of the …rst row of both two dimensional IRs vanish at the planes [010] and [001] and the basis functions of the second rows vanish at the planes [100] and [001]. Of course any linear combination of these functions is also basis function having the same nodal structure. If we take the sum of basis function $E_g(B_{2g})$ + $E_g(B_{3g})$ additional lines of nodes appear in the plane [110]. The linear combination with minus sign has nodes in the plane [110]. It should be noted that point group approach also results di¤erent nodal structure of di¤erent two-dimensional IRs [4] .

3 Discussion of the results

3.1 High-T_c superconductors

The analysis of broad set of experimental data on the of high-T_c superconductors [1] led the most of the authors to the conclusion of singlet pairing and A_g SOP symmetry in these compounds. Angular resolved photoelectron spectra of high-T_c superconductors [29] reveal a strong trough in the diagonal of xy plane indicating $d_{x^2 ¡ y^2}$ pairing with line of nodes . On the other hand some experiments reveal also totally symmetric s pairing without nodes. In many cases an interplay between these two types of pairing [1] both belonging to A_g IR exists. It is seen from tables 2 and 4, that A_g pairing function, obtained group theoretically is noddles and that other IRs have nodes in the coordinate planes only. Hence it follows that nodal structure high-T_c superconductors is more complex then that which follows from the symmetry only. To explain this one can consider two wave vectors $\vec{k}_\alpha$ and $\vec{k}_\beta$ symmetrical with respect to diagonal of the deformed square (Note that the orthorombicity [(b-a)/(b+a)] of YBCuO is about 2 % only [1]).. Two types of basis functions of Cooper pairs belonging to A_g IR $©^s_\alpha$ and $©^s_\beta$ are easily

obtained from the Table 4 by introducing additional subscripts α and β. One can suppose that due to the interaction two self-vectors are linear combinations of these basis states :

$$\mathbb{C}_s^S = C_\alpha \left(\mathbb{C}_{1,\alpha}^S + \mathbb{C}_{2,\alpha}^S + \mathbb{C}_{3,\alpha}^S + \mathbb{C}_{4,\alpha}^S \right) + C_\beta \left(\mathbb{C}_{1,\beta}^S + \mathbb{C}_{2,\beta}^S + \mathbb{C}_{3,\beta}^S + \mathbb{C}_{4,\beta}^S \right) \quad (24)$$

$$\mathbb{C}_{x^2-y^2}^S = C_\beta \left(\mathbb{C}_{1,\alpha}^S + \mathbb{C}_{2,\alpha}^S + \mathbb{C}_{3,\alpha}^S + \mathbb{C}_{4,\alpha}^S \right) - C_\alpha \left(\mathbb{C}_{1,\beta}^S + \mathbb{C}_{2,\beta}^S + \mathbb{C}_{3,\beta}^S + \mathbb{C}_{4,\beta}^S \right) \quad (25)$$

Both combinations belong to IR A_g.of group D_{2h}. First one corresponds to the noddles s-pairing and the second to the $d_{x^2-y^2}$ pairing with line of nodes in the diagonal direction xy-plane . In the limit of zero orthorombic distortion the symmetry group is D_{4h} and $C_\alpha = C_\beta$, subscripts α and β are dropped and the sums in second brackets in right hand sides of (24) and (25) are written as $\mathbb{C}_{13}^S + \mathbb{C}_{14}^S + \mathbb{C}_{15}^S + \mathbb{C}_{16}^S$. In this case combination (24) belongs to IR A_{1g} and combination (25) belongs to IR B_{1g} of the symmetry group D_{4h}. Hence it follows that the nodal structure of SOP in high- T_c superconductors is de…ned by hidden symmetry D_{4h}.

3.2 Antiferromagnetic and ferromagnetic structures

To obtain all possible pairing states in a strong orbit coupling case one should take into account two directions of spin connected at general point of a Brillouin zone by time-reversal only (Kramers degeneration). This can be done by making use antisymmetrized Kronecker square of double valued corepresentations [21] . This procedure results a character (χ_{normal}) corresponding to all possible pairing states in normal state of the crystal. The phase transition to ferromagnetic state may be described as time-reversal symmetry breaking. The character of this state equals to the antisymmetrized square of double valued IR of the space group. Similar state with opposite direction of spins has the same character. In antiferromagnetic state the spins of two electrons are opposite and its total character is written as [21]

$$\chi_{aitif} = \chi_{normal} - 2\chi_{ferro} \quad (26)$$

This direct calculation shows that ferromagnetic state is always odd , but antiferromagnetic states may be even and odd states [21]. Violations of these results are not known to the author so far.

The antisymmetrized Kronecker squares of double-valued IRs and corepresentations for group D_{6h}^4 (symmetry group of UPt_3) of are presented in Table 6. Starting from the general point of the Brillouin zone where all IRs of any parity are possible we are able to enumerate all directions and planes, where some IR is absent and thus indicate point and line nodes of the SOP. For the lines of symmetry, the Kronecker square depends on the index of the small IR and the symmetry analysis depends on the symmetry of the one-electron state. There are two double valued IRs on the planes of symmetry, but their Kronecker squares are the same. Thus on the planes of symmetry the results of the space-group approach to the SOP do not depend on any choice of basis functions.

Table 6.

Possible IRs of Cooper pair of the space group D_{6h}^4.

state	$k(H)$,IR	IRs of Cooper pair
	direction	
	¢ (C_{6v})	
all	p_1, p_2	A_{1g} + A_{1u} + E_{1u}
	p_3	A_{1g} + A_{1u} + B_{1u} + B_{2u}
	planes	
Ferromagnetic odd	¡ KM[1)]	A_{1u} + A_{2u} + 2E_{2u}
Antiferromagnetic odd		B_{1u} + B_{2u} + 2E_{1u}
Antiferromagnetic even		A_{1g} + A_{2g} + 2E_{2g}
normal		All IRs except E_{1g},B_{1g} and B_{2g}
Ferromagnetic odd	¡ ML[2)]	A_{1u} + B_{2u} + E_{1u} + E_{2u}
Antiferromagnetic odd		A_{2u} + B_{1u} + E_{1u} + E_{2u}
Antiferromagnetic even		A_{1g} + B_{2g} + E_{1g} + E_{2g}
normal		All IRs except A_{2g} and B_{1g}
Ferromagnetic odd	¡ KH[3)]	A_{1u} + B_{1u} + E_{1u} + E_{2u}
Antiferromagnetic odd		A_{2u} + B_{2u} + E_{1u} + E_{2u}
Antiferromagnetic even		A_{1g} + B_{1g} + E_{1g} + E_{2g}
normal		All IRs except A_{2g} and B_{2g}

[1)] Basal plane

[2)] Vertical plane perpendicular to the lateral face of Brillouin zone

[3)] Vertical plane passing via lateral edge of Brillouin zone

Some of the existing models of superconductivity of UPt_3 connect the double superconducting transition which is seen in heat capacity [30] and ultrasonic attenuation [31] experiments in a magnetic …eld, with two-dimensionality of the SOP. The E_{1u} model was proposed in Refs. [32, 33] . The E_2 and E_{2u} models were proposed in Refs. [34] and [35, 36] respectively. An E_{1g} model was considered in Ref. [37]. The second type of models connects the double superconducting transition with two one-dimensional IRs. In Ref. [38]. the scenario [42]of a superconducting transition based on the IR A_{2u} , whose degeneracy is lifted by spin-orbit coupling, was developed, but the possibilities of B_{1u} and B_{2u} were also considered. The model of Ref. [39] is based on the idea of two nearly degenerated one-dimentsional representations A and B. The scenario of superconducting transition in UPt_3 based on IRs A_{1u} and A_{2u} was proposed in Ref. .[40] The third type of model is based on both types of IRs - one-dimensional and two-dimensional. The singlet pairing based on the IRs A_{1g} and E_{1g} was also considered in Ref. [40] . The model of Ref. [41] includes the A_1 + E_1 symmetry of the superconducting state. Thus almost all the IRs and several their combinations have been discussed as possible candidate for the description of the superconducting state in UPt_3.

We are in position to show how the space-group approach makes it possible to …nd the symmetry of SOP, which corresponds to the experimental data. UPt_3 is an antiferromagnetic superconductor [42] with odd SOP [43] , so we limit our consideration of Table 6 to the odd IRs corresponding to antiferromagnetic phase. Experimental data .[44] indicate a line of nodes in the basal plane and hence it follows from the Table 6 that IRs A_{1u}, A_{2u} and E_{2u} are appropriate candidates. Experiments [44] also indicate point node (nodes) in vertical direction and IR A_{1u} having lines of nodes in two sets of vertical planes should be excluded. Both remaining IRs E_{2u} and A_{2u} have point nodes in vertical direction and are appropriate candidates. The double superconducting transition in UPt_3 is usually connected with the two-dimensionality of SOP (see e.g. [44]) and we adopt this point in the present work. Hence we conclude from the data of Table 6, that there is an agreement with all experimental data for the IR E_{2u} only.

It should be also noted that the analysis of recent experiments on anisotropic magnetization

of superconducting UPt_3 [45] leaved two possibilities for SOP: E_{1g} and E_{2u}. It follows from the Table 6 that the nodal structure of these two IRs is the same, but the assumption of the odd one is in agreement with Knight shift experiments [43, 46]. Hence it follows the result of our theoretical analysis of experimental data is in agreement with the results of Refs. [34, 35, 36, 45].

It should be emphasized that the corollary of the Frobenius reciprocity theorem that two-dimensional IRs appear twice is reinforced by the double superconducting transition in UPt_3 [9].(Note that it is not a pure mathematical fact, bur consequence of conservation of total space dimension of two one-electron states in the two-electron state). In our approach two almost degenerate E_{2u} states interact forming two self-vectors, corresponding to two superconducting transitions.

Possible applications of the developed technique to recently discovered ferromagnetic superconductors should be also discussed. Muon spin-relaxation experiments [47] on the superconducting Sr_2RuO_4 reveal spontaneous appearance of internal magnetic …eld below the transition temperature: the appearance of such a …eld indicates that the superconducting state in this material is characterized by the breaking of time-reversal symmetry. Knight-shift measurements of Sr_2RuO_4 using ^{17}O NMR show no change in spin susceptibility on passing through the superconducting transition temperature, which provides the de…nitive identi…cation of Sr_2RuO_4 as a spin-triplet (odd-parity) superconductor [48].

As a …rst approximation ferromagnetic ‡uctuations can be described as removing of time-reversal from the symmetry group [27]. On the other hand, all Shubnikov groups compatible with ferromagnetism are already enumerated, leaving only one possibility, namely $4/mm0m0$ for ferromagnetic superconductor with D_{4h} point group [49].

The space-group approach can be easily generalized on strong spin-orbit coupling case and Shubnikov groups of type III making use of the spin-space-group approach of Brinkman and Elliott [50] as follows. The left coset representatives in formula (7) act also on the spin part of Anderson function . If any of the point operations is associated with time-reversal, the directions of spins in a pair are reversed.

3.3 Conclusion

Space group approach to the wavefunction of a Cooper pair is developed with projection operator technique and applied to construction of Cooper pair wavefunction In D_{2h} and D_{4h} symmetries relevant to high-T_c superconductors. The nodal structure of SOP is obtained and discussed for D_{2h} , D_{4h} and D_{6h} symmetries. It is shown that violations of Blount theorem accompany symmetry breaking to axial point groups. It restless in appearance of lines of nodes for triplet SOP in strong spin-orbit coupling case. It is obtained that experimentally observe nodal structure of SOP in high-T_c superconductors follow from the hidden symmetry D_{4h}.

The theoretical results for D_{6h} are used to analyze experimental data for antiferromagnetic superconductor UPt_3 and it is proposed that superconductivity in this HF compound is de…ned by the SOP corresponding to two almost degenerate E_{2u} IR.

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4 Appendix

In appendix we present for convenience of reader Kovalev's [25]. notations of group operators and part of group multiplication table, which is used for nodal structure analysis. In this notations for O_h group the element $h_1 ... h_{24}$ correspond to pure rotations , h_{25} is the space inversion and the elements $h_{25} ... h_{48}$ are left cosets by space inversion as follows

$$h_{25} \cdot h_i = h_{i+24} \quad ,1 \cdot i \cdot 24 \tag{27}$$

and:

$$h_{25} \cdot h_j = h_{j\,|\,24} \quad ,25 \cdot J \cdot 48 \tag{28}$$

Table A1. Kovalev's notations of the elements of D_{4h} group

	operation	angle	axis		operation	axis
h_1	identity			h_{25}	inversion	
h_2	rotation	$180^{\pm}$	[100]	h_{26}	re‡ection	[100]
h_3	rotation	$180^{\pm}$	[010]	h_{27}	re‡ection	[010]
h_4	rotation	$180^{\pm}$	[001]	h_{28}	re‡ection	[001]
h_{13}	rotation	180^{o}	$[\bar{1}10]$	h_{37}	re‡ection	$[\bar{1}10]$
h_{14}	rotation	90^{o}	[001]	h_{38}	$I \pounds h_{14}$	
h_{15}	rotation	270^{o}	[001]	h_{39}	$I \pounds h_{15}$	
h_{16}	rotation	180^{o}	[110]	h_{40}	re‡ection	[110]

To envisage the analysis of nodal structure of SOP we present also part of group multiplication table [25], representing the action of re‡ections on spatial part of singlet Anderson function. Note that for triplet function the minus sign should be added in all cases.

Table A2. Mirror counterparts of singlet Anderson functions.
(obtained by the action of the operators of the …rst row on the functions of the …rst column.)

	h_{26}	h_{27}	h_{28}	h_{37}	h_{40}
$©_1^s$	$©_2^s$	$©_3^s$	$©_4^s$	$©_{13}^s$	$©_{16}^s$
$©_2^s$	$©_1^s$	$©_4^s$	$©_3^s$	$©_{14}^s$	$©_{15}^s$
$©_3^s$	$©_4^s$	$©_1^s$	$©_2^s$	$©_{15}^s$	$©_{14}^s$
$©_4^s$	$©_3^s$	$©_2^s$	$©_1^s$	$©_{16}^s$	$©_{13}^s$
$©_{13}^s$	$©_{14}^s$	$©_{15}^s$	$©_{16}^s$	$©_1^s$	$©_4^s$
$©_{14}^s$	$©_{13}^s$	$©_{16}^s$	$©_{15}^s$	$©_3^s$	$©_2^s$
$©_{15}^s$	$©_{16}^s$	$©_{13}^s$	$©_{14}^s$	$©_2^s$	$©_3^s$
$©_{16}^s$	$©_{15}^s$	$©_{14}^s$	$©_{13}^s$	$©_4^s$	$©_1^s$