IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Space group approach to the wavefunction of a Cooper pair

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1992 J. Phys.: Condens. Matter 4 3525

(http://iopscience.iop.org/0953-8984/4/13/015)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.159
The article was downloaded on 12/05/2010 at 11:38

Please note that terms and conditions apply.

J. Phys.: Condens. Matter 4 (1992) 3525–3532. Printed in the UK

Space group approach to the wavefunction of a Cooper pair

V G Yarzhemsky† and E N Murav'ev‡
† Karpov Institute of Physical Chemistry, ul. Obukha 10, Moscow 103064, Russia
‡ Kurnakov Institute of General and Inorganic Chemistry, Leninski Pr. 31, Moscow 117907, Russia

Received 24 June 1991, in final form 28 November 1991

Abstract. The method of construction of the wavefunction of a Cooper pair based on the Pauli exclusion principle and the Mackey–Bradley theorem is developed. Tables of symmetrized and antisymmetrized Kronecker squares of single- and double-valued irreducible representations of the groups O_h^6 and D_{6h}^4 are obtained. The tables are used to search for points in the Brillouin zone where totally symmetric Cooper pairs can exist. It is shown that, in the symmetrical points and directions in a Brillouin zone, a direct connection between the multiplicity and parity of the Cooper pair wavefunction does not exist.

1. Introduction

Group theoretical approaches to the wavefunction of a Cooper pair are mainly due to Anderson (1959, 1984) and Anderson and Morel (1961). Anderson (1959) pointed out the time inversion connection between the wavefunctions of the electrons in a singlet pair. The total momentum and spin of such a pair are equal to zero, and its wavefunction belongs to the totally symmetric irreducible representation (IR) A_{1g}. Anderson and Morel (1961) pointed out the possibility of condensation of fermion pairs with non-zero total orbital momentum in liquid ^{3}He and transition metals. After the discovery of heavy-fermion superconductors with probable triplet Cooper pairing, the theory was generalized. According to Anderson's (1984) approach, the wavefunctions of electrons in a triplet Cooper pair may be connected by time and space inversion and the product of these operations. In this approximation the orbital part of a triplet pair is odd (ungerade) and orbital part of a singlet pair is even (gerade). It is obvious that when symmetry is reduced to crystal point group with inversion, the parity of the wavefunction is conserved.

Volovik and Gor'kov (1985) and Blount (1985) also pointed out that the orbital part of a triplet pair is odd and one of a singlet pair is even. They considered the subgroups of O_h, D_{6h} and D_{4h} point symmetries, where the superconducting order parameter belongs to the one-dimensional IR. The same results on the superconducting order parameter were obtained by Ozaki and Machida (1989). Ueda and Rice (1985) investigated the influence of spin–orbit coupling on the symmetry of the superconducting order parameter in point symmetry O. Sigrist and Rice (1987) classified symmetries of superconducting states in high-T_c superconductors with and without spin–coupling. The authors of all the above-mentioned theories used a point group approach to describe the wavefunction of a Cooper pair and the superconducting order parameter. In this case the spin part of the wavefunction of a Cooper pair belongs to an even IR, and it is obvious that in the *L–S* coupling approximation, the total wavefunction of a triplet Cooper pair (i.e. the direct product of its spin and orbital parts) will never belong to the totally symmetric A_{1g} IR. We shall show below that, in a space group approach, totally symmetric triplet Cooper pairs can exist in some points or directions in Brillouin zone without any symmetry reduction.

Izyumov *et al* (1989) suggested constructing the wavefunction of a Cooper pair as a direct (Kronecker) product of electron wavefunctions belonging to the space group IR. They proposed that in a space group approach the direct connection between multiplicity and parity of a Cooper pair may be not valid in some symmetrical points of a one-electron Brillouin zone. Yarzhemsky (1990) showed that this approach must be used in time-reversal symmetry breaking and applied the Pauli exclusion principle. According to the Pauli exclusion principle, the orbital part of a singlet pair belongs to the symmetrized Kronecker square and the orbital part of a triplet pair belongs to the antisymmetrized Kronecker square. It should be emphasized that the symmetrized and antisymmetrized Kronecker squares of IRs for the groups O_h^5 and O_h^7 obtained by Birman (1974) may be used for the symmetry group O_h^6 of the heavy-fermion superconductor UBe_{13}, if the wavevector $\boldsymbol{k}$ is inside the Brillouin zone. So we can see from Birman's (1974) tables that the above-mentioned direct connection between multiplicity and parity of the wavefunction of a Cooper pair is violated in some symmetrical directions in the Brillouin zone, when we change from point groups to real space groups. The latter statement is in agreement with the proposition of Izyumov *et al* (1989).

The present work is aimed at elucidating the consequences of permutation symmetry and the structure of the space group on the symmetry of the wavefunction of the Cooper pair. We construct the wavefunction of a Cooper pair, making use of the Pauli exclusion principle and Mackey's (1953) theorem on the symmetrized and antisymmetrized squares of induced representations. We present the tables of symmetrized and antisymmetrized Kronecker squares of single-valued and double-valued IRs for the symmetry groups O_h^6 and D_{6h}^4 of heavy-fermion superconductors UBe_{13} and UPt_3, respectively. The crystal structures of these superconductors correspond to the data reported by Ozaki and Machida (1989). The tables are used to search for points and directions in a Brillouin zone, where totally symmetric (A_{1g}) singlet and triplet Cooper pairs can exist without any symmetry violation of the crystal. *L–S* and *j–j* coupling approximations are considered.

2. Theory

We show briefly how the physical problem that we are treating leads inevitably to the mathematical methods mentioned above. The wavefunction of a double-electron state is constructed as a direct (Kronecker) product of one-electron wavefunctions. If these electrons are equivalent, the requirement of antisymmetry of the total wavefunction permits us to carry out the partial reduction in the total wavefunction and to obtain symmetries of singlet and triplet states. We can do no more than to consider a Cooper pair in a solid as a state of two equivalent electrons obeying the Pauli exclusion principle. So in the *L–S* coupling approximation the antisymmetrized Kronecker square of the spin part of the wavefunction (singlet pair) is combined with the symmetrized Kronecker

Table 1. The Kronecker squares of IRs of group O_h^6 (only parts with zero total momentum are included). The points and directions in a Brillouin zone are marked according to figure 1. The symmetrized square is for the singlet pair in *L–S* coupling; the antisymmetrized square is for the triplet pair in *L–S* coupling and for the pair in *j–j* coupling. Kovalev's (1986) notation is used for the single-valued IRs (t_i) and the double-valued IRs (p_i) of the wavevector group. The spectroscopic notation is used for IRs at point Γ (Hammermesh 1964, Kovalev 1986).

Wavevector subgroup IR	Symmetrized square IR	Antisymmetrized square IR
X′ (D_{4h})		
t_1–t_8	$A_{1g} + E_g$	—
t_9, t_{10}	$A_{1g} + A_{2g} + 2E_g + T_{2g}$	T_{1g}
p_1–p_4	$2T_{1g} + T_{2g}$	$A_{1g} + E_g$
Δ′ (C_{4v})		
t_1–t_4	$A_{1g} + E_g$	T_{1u}
t_5	$A_{1g} + A_{1u} + A_{2u} + 2E_g + E_u + T_{2g}$	$A_{2u} + E_u + T_{1g} + T_{1u} + T_{2u}$
p_1, p_2	$2T_{1g} + T_{1u} + T_{1g}$	$A_{1g} + A_{1u} + E_g + E_u + T_{1u} + T_{2u}$
L (D_{3d})		
t_1	$A_{1g} + A_{1u} + A_{2g} + T_{1g} + T_{2g} + T_{2u}$	$A_{2u} + T_{1u}$
t_2, t_3	$A_{1u} + E_g + T_{1g} + T_{2g} + T_{2u}$	$A_{2u} + T_{1u}$
p_1	$A_{1g} + A_{2g} + A_{2u} + T_{1g} + T_{1u} + T_{2g}$	$A_{1u} + T_{2u}$
p_2, p_3	$A_{2u} + E_g + T_{1g} + T_{1u} + T_{2g}$	$A_{1u} + T_{2u}$
Λ (C_{3v})		
t_1, t_2	$A_{1g} + T_{2g}$	$A_{2u} + T_{1u}$
t_3	$A_{1g} + A_{1u} + E_g + T_{1g} + 2T_{2g} + T_{2u}$	$A_{2g} + A_{2u} + E_u + T_{1g} + 2T_{1u} + T_{2u}$
p_1, p_2	$A_{2g} + T_{1g}$	$A_{1u} + T_{2u}$
p_3	$A_{2g} + A_{2u} + E_g + 2T_{1g} + T_{1u} + T_{2g}$	$A_{1g} + A_{1u} + E_u + T_{1u} + T_{2g} + 2T_{2u}$
Σ (C_{2v})		
t_1–t_4	$A_{1g} + E_g + T_{2g}$	$T_{2u} + T_{1u}$
p	$A_{2g} + E_g + 3T_{1g} + T_{1u} + 2T_{2g} + T_{2u}$	$A_{1g} + A_{1u} + A_{2u} + E_g + 2E_u + 2T_{2u} + 2T_{1u} + T_{2g}$

square of an orbital part of the wavefunction and the symmetrized square of the spin part (triplet pair) is combined with antisymmetrized square of the orbital part. In the *j–j* coupling approximation the wavefunction of a Cooper pair belongs to the antisymmetrized Kronecker square of the double-valued IR of the space group.

In this section we consider the *L–S* coupling only, but the results on the *j–j* coupling are included in tables 1 and 2. In this case the orbital components of the wavefunctions of the electrons in a Cooper pair belong to IRs of the crystal space group. We investigate properly only the case when the spin part of the wavefunction belongs to space groups IRs in the centre of the Brillouin zone (Γ point), i.e. double-valued IRs of the point group, but tables 1 and 2 can be used for all types of spin wavefunctions. When symmetrizing characters of double-valued IRs of point groups, we may easily obtain IRs of the spin components of triplet pairs T_{1g} and $E_{1g} + A_{2g}$ for groups O_h and D_{6h} respectively. The spin components of singlet pairs belong to IRs A_{1g} for both groups.

In real crystals the orbital component of the electron wavefunction in the *L–S* approximation and the total wavefunction in the *j–j* approximation belong to the single-valued or double-valued IR of the space group. According to Bradley and Cracknell (1972) and Altman (1977) the IRs of the space group *G* are obtained by the induction of

Table 2. Kronecker squares of IRs of group D^1_{6h} (*only parts with zero total momentum are included*). The points and directions in a Brillouin zone are marked according to figure 2. The other notation is as for table 1.

Wavevector subgroup IR	Symmetrized square IR	Antisymmetrized square IR
A (D_{6h})		
t_1, t_2	$A_{1g} + B_{1g} + B_{2u}$	A_{2u}
t_3	$A_{1g} + A_{1u} + B_{1g} + B_{2u} + E_{1g} + E_{1u} + E_{2g}$	$A_{2g} + A_{2u} + B_{1u} + B_{2g} + E_{2u}$
p_1, p_2	$A_{2g} + A_{2u} + B_{2g}$	B_{2u}
p_3	$A_{2g} + A_{2u} + B_{1u} + B_{2g} + E_{1g} + E_{2g} + E_{2u}$	$A_{1g} + A_{1u} + B_{1g} + B_{2u} + E_{1u}$
Δ (C_{6v})		
t_1–t_4	A_{1g}	A_{2u}
t_5, t_6	$A_{1g} + A_{1u} + E_{2g}$	$A_{2g} + A_{2u} + E_{2u}$
p_1, p_2	$A_{2g} + A_{2u} + E_{1g}$	$A_{1g} + A_{1u} + E_{1u}$
p_3	$A_{2g} + A_{2u} + B_{1g} + B_{2g}$	$A_{1g} + A_{1u} + B_{1u} + B_{2u}$
M (D_{2h})		
t_1–t_8	$A_{1g} + E_{2g}$	—
p_1, p_2	$A_{2g} + B_{1g} + B_{2g} + 2E_{1g} + E_{2g}$	$A_{1g} + E_{2g}$
Σ (C_{2V})		
t_1–t_4	$A_{1g} + E_{2g}$	$B_{2u} + E_{1u}$
p	$A_{2g} + B_{1g} + B_{2g} + B_{2u} + 2E_{1g} + E_{1u} + E_{2g}$	$A_{1g} + A_{1u} + A_{2u} + B_{1u} + E_{1u} + E_{2g} + 2E_{2u}$
L (D_{2h})		
t_1, t_2	$A_{1g} + B_{1g} + B_{2u} + E_{1g} + E_{1u} + E_{2g}$	$A_{2u} + E_{2u}$
p_1, p_2	$A_{2g} + A_{2u} + B_{2g} + E_{1g} + E_{2g} + E_{2u}$	$B_{2u} + E_{1u}$
K (D_{3h})		
t_1–t_4	A_{1g}	B_{1u}
t_5, t_6	$A_{1g} + B_{2u} + E_{2g}$	$A_{2g} + B_{1u} + E_{1u}$
p_1	$A_{2g} + B_{1g} + B_{1u} + B_{2g}$	$A_{1g} + A_{1u} + A_{2u} + B_{2u}$
p_2, p_3	$A_{2g} + B_{1u} + E_{1g}$	$A_{1g} + B_{2u} + E_{2u}$
T (C_{2v})		
t_1–t_4	$A_{1g} + E_{2g}$	$B_{1u} + E_{1u}$
p	$A_{2g} + B_{1g} + B_{1u} + B_{2g} + 2E_{1g} + E_{1u} + E_{2g}$	$A_{1g} + A_{1u} + A_{2u} + B_{2u} + E_{1u} + E_{2g} + 2E_{2u}$
H (D_{3h})		
t_1	$A_{1g} + B_{1g} + B_{2g} + B_{2u}$	$A_{1u} + A_{2g} + A_{2u} + B_{1u}$
t_2, t_3	$A_{1g} + B_{2u} + E_{1g}$	$A_{2g} + B_{1u} + E_{2u}$
p_1–p_4	A_{2g}	B_{2u}
p_5, p_6	$A_{2g} + B_{1u} + E_{2g}$	$A_{1g} + B_{2u} + E_{1u}$

IRs D^k (small IRs) of the wavevector k group H (subgroup) into the space group. We denote these IRs according to Bradley and Cracknell (1972) as $D^k \uparrow G$. The method of the decomposition of Kronecker squares of induced representations into symmetrized and antisymmetrized parts was developed by Mackey (1953), and applied to space groups by Bradley and Davies (1970). Let us consider the main statements of the Mackey–Bradley theorem and its application to Cooper pairing.

The structure of the Kronecker square of an induced IR may be easily envisaged by the double coset decomposition of G relative to H which is written as

$$G = \sum_{\sigma} H d_\sigma H. \tag{1}$$

For every d_σ in (1) including the identity element d_1 we introduce the subgroup $M_\sigma = H \cap d_\sigma H d_\sigma^{-1}$ and consider its representation, given by the formula

$$P_\sigma = D^k(m) \otimes D^k(d_\sigma^{-1} m d_\sigma). \tag{2}$$

The wavevector $\boldsymbol{k}_\sigma$ of this representation is defined by the relation

$$\boldsymbol{k} + d_\sigma \boldsymbol{k} = \boldsymbol{k}_\sigma + \boldsymbol{b}_\sigma \tag{3}$$

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

If α is a self-inverse double coset (i.e. $H d_\alpha H = H d_\alpha^{-1} H$) there are two extensions of P_α into subgroup $M_\alpha^* = M_\alpha + a M_\alpha$, which are defined by their characters as

$$\chi(P_\alpha^+(am)) = \chi(D^k(amam)) \tag{4}$$

$$\chi(P_\alpha^-(am)) = -\chi(D^k(amam)) \tag{5}$$

where

$$a = d_\alpha h_1 = h_2 d_\alpha \qquad (h_1, h_2 \in H). \tag{6}$$

Then the symmetrized and antisymmetrized parts of the Kronecker square of the induced representation (in our case the IR $D^k \uparrow G$ of the space group) are given by the two following formulae:

$$[(D^k \uparrow G) \otimes (D^k \uparrow G)] = [D^k \otimes D^k] \uparrow G + \sum_{\alpha} P_\alpha^+ \uparrow G + \sum_{\beta} P_\beta \uparrow G \tag{7}$$

$$\{(D^k \uparrow G) \otimes (D^k \uparrow G)\} = \{D^k \otimes D^k\} \uparrow G + \sum_{\alpha} P_\alpha^- \uparrow G + \sum_{\beta} P_\beta \uparrow G. \tag{8}$$

The first items on the right-hand sides of (7) and (8) correspond to the double coset defined by the identity element. The summations in the second items on the right-hand sides of (7) and (8) run over all self-inverse double cosets α. Index β in the last summations on the right-hand sides of (7) and (8) corresponds to couples of non-self-inverse double cosets $H d_\beta H \neq H d_\beta^{-1} H$. According to the Pauli exclusion principle the symmetrized Kronecker square (equation (7)) defines the orbital part of the singlet state (antisymmetrized with respect to spin coordinates) and the antisymmetrized Kronecker square (equation (8)) defines the orbital part of the triplet state (symmetrized with respect to spin coordinates). It follows from the Mackey–Bradley theorem that the symmetries of these states are different for identity and self-inverse double cosets and are the same for non-self-inverse double cosets. This does not mean of course that the same IRs cannot appear in the decomposition of the two first items on the right-hand sides in equations (7) and (8) simultaneously. These double-electron states may correspond to Cooper pairs if the wavevector $\boldsymbol{k}_\sigma$ of a pair which is given by equation (3) equals zero.

We intend now to envisage the dependence of the symmetry of a Cooper pair upon its multiplicity and the value of the one-electron wavevector. If the one-electron wavevector is in the centre of the Brillouin zone, we have only one double coset, defined by the identity element and we may use the theory of point group IRs (Hamermesh 1964). It is obvious that in this case both the singlet and the triplet pairs have even orbital parts. The antisymmetrized squares for the one-dimensional IRs vanish, and therefore triplet pairs are forbidden. If the one-electron wavevector equals the half-integer vector of the reciprocal lattice, the wavevector of a Cooper pair given by equation (3) equals zero for the identity double coset. It follows from equations (7) and (8) that, if space inversion belongs to H, we get only even IRs of H for symmorphic space groups in this case. However, if the space group is non-symmorphic, additional phase multipliers arise in the decomposition of the Kronecker square (Murav'ev and Yarzhemsky 1986) and even and odd IRs of H will be mixed in the decomposition of symmetrized and antisymmetrized squares. It is clear that, when we induce IRs from H to G, the parity of representation is conserved. Hence it follows that, if the one-electron wavevector equals the half-integer vector of the reciprocal lattice and the space group is symmorphic, the orbital parts of the triplet and singlet Cooper pairs are even, but the direct connection between multiplicity and parity of the wavefunction of the Cooper pair does not exist for non-symmorphic space groups in this case.

We are now in a position to use the Mackey–Bradley theorem and to investigate the validity of the proposition of Izyumov *et al* (1989) that the direct connection between multiplicity and parity of the wavefunction of a Cooper may be violated for two-dimensional small IRs inside the Brillouin zone. Let us consider the case of non-equivalent vectors $\boldsymbol{k}$ and $-\boldsymbol{k}$ inside the Brillouin zone. In this case we can take space inversion as a representative element of the self-inverse double coset. As follows from equation (3), the total momentum of such a pair is equal to zero. The signs of the representations P_α^+ and P_α^- defined by equations (4) and (5) are opposite if the group element belongs to the left coset defined by space inversion, but this does not mean that P_α^+ and P_α^- may be decomposed onto IRs of opposite parity. Let us consider two cases. If the IR is two dimensional, the two characters of P_α^+ and P_α^- for the identity element are equal to 4. It follows from equations (4) and (5) that the characters of P_α^+ and P_α^- for inversion equal to 2 and -2, respectively. It is obvious that in this case both even and odd IRs will be mixed in the decomposition of $P_\alpha^+ \uparrow G$ and $P_\alpha^- \uparrow G$. Another case takes place if the IR is one dimensional and the characters are such that $\chi^2(D^k(m)) = 1$ and $\chi(D^k(m^2)) = 1$. In this case the character for the left coset defined by inversion is equal to 1 in the representation P_α^+ and to -1 in the representation P_α^-. It follows that $P_\alpha^+ \uparrow G$ is decomposed on the even IR of G, and $P_\alpha^- \uparrow G$ on the odd IRs only. If group H consists of the identity element only, we may easily deduce from equations (4) and (5) and the Frobenius reciprocity theorem that $P_\alpha^+ \uparrow G$ contains only even IRs and $P_\alpha^- \uparrow G$ only odd IRs of G. The frequency of appearance of each representation is equal to its dimension. Therefore, in a space group approach the wavefunction of a singlet pair is even and the wavefunction of a triplet pair is odd if the k-vector of the electron belongs to a non-symmetric direction inside the Brillouin zone.

The decompositions of Kronecker squares of IRs of space groups O_h^6 and D_{6h}^4 are given in tables 1 and 2, respectively. Kovalev (1965, 1986) projective single-valued and double-valued IRs t_i and p_i are used for small IRs. The Brillouin zones are shown in figures 1 and 2.

3. Discussion

According to Volovik and Gor'kov (1985), the total Cooper pair wavefunction is the superconducting order parameter. From tables 1 and 2 we can find points in the Brillouin zone and small one-electron IRs for which a superconducting phase transition is possible in the space groups under consideration. The spin function of a singlet pair belongs to IR A_{1g} in both groups. The total wavefunction in the L–S coupling approximation is a

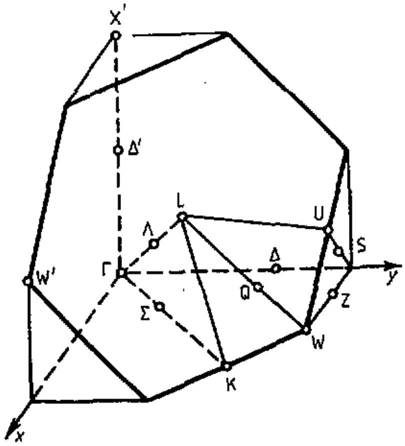

Figure 1. Brillouin zone for the Cf lattice (space group, O_h^6). The points and directions are marked according to Kovalev (1986).

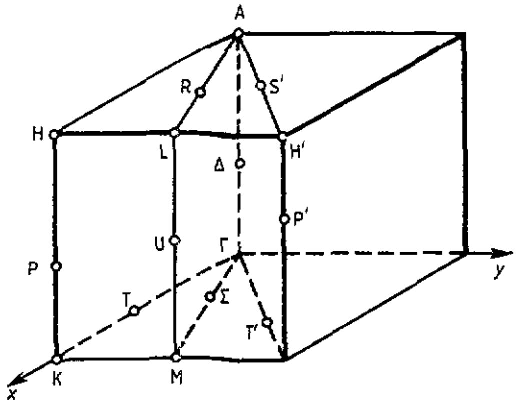

Figure 2. Brillouin zone for the H lattice (space group, D_{6h}^4). The points and directions are marked according to Kovalev (1986).

direct product of orbital and spin parts. It follows that the superconducting order parameter of the singlet pair is totally symmetric, if the symmetrized Kronecker square of the orbital component of the wavefunction belongs to IR A_{1g}. It is seen from tables 1 and 2 that totally symmetric singlet Cooper pairs can exist in all the IRs considered, except IRs $t_2(L)$ and $t_3(L)$ of group O_h^6. (We indicate the point or direction in the Brillouin zone in parentheses.) The spin part of the triplet pair belongs to IRs T_{1g} in the O_h^6 group and to $E_{1g} + A_{2g}$ in the D_{6h}^4 group. So totally symmetric triplet Cooper pairs are possible if these IRs appear in the antisymmetrized square of the orbital part. It is seen from tables 1 and 2 that this is the case for the two-dimensional small IRs $t_9(X')$, $t_{10}(X')$, $t_5(\Delta')$ and $t_3(\Lambda)$ in group O_h^6 and for the two-dimensional small IRs $t_3(A)$, $t_5(A)$, $t_6(\Delta)$, $t_5(K)$, $t_6(K)$ and $t_1(H)$, $t_2(H)$ and $t_3(H)$ in group D_{6h}^4. It is obvious from the evidence given in the previous section that, in non-symmetric points inside the Brillouin zone, singlet pairs with A_{1g} symmetry are always possible but totally symmetric triplet pairs are forbidden.

The criterion of existence of totally symmetric Cooper pairs in the *j–j* approximation is quite straightforward: the antisymmetrized Kronecker square of the double-valued IR of space group includes A_{1g} IR. From tables 1 and 2, we come to the conclusion that totally symmetric Cooper pairs are possible for all double-valued IRs considered in O_h^6 group except point L and one-dimensional IRs $p_1(\Lambda)$ and $p_2(\Lambda)$. In the D_{6h}^4 group we have A_{1g} in the antisymmetrized square of all double-valued IRs considered except the IRs $p_1(L)$, $p_2(L)$, $p_1(H)$, $p_2(H)$, $p_3(H)$, $p_4(H)$, $p_1(A)$ and $p_2(A)$. In non-symmetric points of the Brillouin zone, the antisymmetrized square of the double-valued IR contains only odd IRs and, in the *j–j* coupling approximation, totally symmetric Cooper pairs are forbidden.

4. Conclusion

In the case of real crystals the space group approach is a quite straightforward generalization of the Anderson (1984) point group approach to the wavefunction of a Cooper pair. We showed that the application of the Mackey–Bradley theorem and the Pauli exclusion principle makes it possible to investigate the symmetry of the wavefunction of a Cooper pair in crystals. In the space group approach the wavefunction of a singlet Cooper pair is even and the wavefunction of a triplet pair is odd if the wavevector of the electron is inside the Brillouin zone and the small IR is one dimensional. This statement is in agreement with the results of Anderson (1984), Volovik and Gor'kov (1985) and Blount (1985), but this direct connection between multiplicity and parity of the wavefunction of a Cooper pair is violated on the surface of the Brillouin zone and for two-dimensional small IRs inside the Brillouin zone. We have obtained tables of symmetrized and antisymmetrized squares with zero total wavevector of IRs for the symmetry groups O_h^6 and D_{6h}^4 of the heavy-fermion superconductors UBe_{13} and UPt_3.

These tables may be used for the symmetry description of Cooper pairs in these materials. In a space group approach, triplet Cooper pairs with totally symmetric (A_{1g}) wavefunction can exist in some symmetrical points and directions in one-electron Brillouin zone without any symmetry violation of a crystal.

Acknowledgments

We sincerely thank Dr A N Sokolov and Dr R D Harcourt for useful discussion of the manuscript.

References

Altman S L 1977 *Induced Representations in Crystals and Molecules* (New York: Academic)
Anderson P W 1959 *J. Phys. Chem. Solids* **11** 26
—— 1984 *Phys. Rev.* B **30** 4000
Anderson P W and Morel P 1961 *Phys. Rev.* **123** 1911
Birman J L 1974 *Theory of Crystal Space Groups and Infra-Red and Raman Lattice Processes of Insulating Crystals* (Berlin: Springer)
Blount E I 1985 *Phys. Rev.* B **32** 2935
Bradley C J and Cracknell A P 1972 *The Mathematical Theory of Symmetry in Solids. Representation Theory of Point Groups and Space Groups* (Oxford: Clarendon)
Bradley C J and Davies B L 1970 *J. Math. Phys.* **11** 1536
Hamermesh M 1964 *Group Theory and Its Application to Physical Problems* (Reading, MA: Addison-Wesley)
Izyumov Y A, Laptev V M and Syromyatnikov V N 1989 *Int. J. Mod. Phys.* **3** 1377
Kovalev O V 1965 *Irreducible Representations of Space Groups* (New York: Gordon & Breach)
—— 1986 *Irreducible Representations and Corepresentations of Fedorov Groups* (Moscow: Nauka) (in Russian)
Mackey G W 1953 *Am. J. Math.* **75** 387
Murav'ev E N and Yarzhemsky V G 1986 *Dokl. Akad. Nauk* **288** 162 (in Russian)
Ozaki M and Machida K 1989 *Phys. Rev.* B **39** 4145
Sigrist M and Rice T M 1987 *Z. Phys.* B **68** 9
Ueda K and Rice T M 1985 *Phys. Rev.* B **31** 7114
Volovik G E and Gor'kov L P 1985 *Zk. Eksp. Teor. Fiz.* **88** 1412 (in Russian)
Yarzhemsky V G 1990 *Supercond.: Phys- Chem. Tech.* **3** 2504 (in Russian)