

Research Article

Induced Representation Method in the Theory of Electron Structure and Superconductivity

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It is shown that the application of theorems of induced representations method, namely, Frobenius reciprocity theorem, transitivity of induction theorem, and Mackey theorem on symmetrized squares, makes simplifying standard techniques in the theory of electron structure and constructing Cooper pair wavefunctions on the basis of one-electron solid-state wavefunctions possible. It is proved that the nodal structure of topological superconductors in the case of multidimensional irreducible representations is defined by additional quantum numbers. The technique is extended on projective representations in the case of nonsymmorphic space groups and examples of applications for topological superconductors $U\text{Pt}_3$ and Sr_2RuO_4 are considered.

1. Introduction

Induced representation method is a powerful group-theoretical technique for the systems with subgroups of symmetry, such as symmetrical clusters and crystals. There are two essential subgroups, namely, local symmetry group of an atom in a cluster or crystal and the wavevector group (little group) in a BZ (Brillouin zone). The induced representation method and its application to crystals and molecules have been described in two classical books of Bradley and Cracknell [1] and Altman [2]. On the basis of this theory, it was recognized that the standard technique for construction of normal vibrations [3–6] and SALCs (symmetry adapted linear combinations) in clusters [6, 7] can be significantly simplified [8–11]. The Mackey theorem on symmetrized squares [12] and its new form for solid-state wavefunctions of Bradley and Davis [13] made the application of Pauli exclusion principle to solid-state wavefunctions possible, easy, and straightforward [14]. It follows from the space-group approach to the wavefunction of a Cooper pair [14, 15] that generally accepted direct relations between multiplicity and parity of a Cooper pair [16] are violated on symmetry axis in a BZ and on surfaces of a BZ in the case of nonsymmorphic space groups. Calculation of Cooper pair functions making

use of the space group approach for $U\text{Pt}_3$ and some other superconductors [17–21] confirmed this statement. It was also shown that transitivity of induction theorem results in additional quantum numbers for nanoclusters [22] and Cooper pairs [23–25].

In the present work, the advantages of induced representation method for normal vibrations and SALCs construction and for the investigations of Cooper pair symmetry in topological superconductors are reviewed and some calculations for topological superconductors are performed. The pair nodal structure dependence on additional quantum number of IR (irreducible representation) E_u of D_{4h} group in x - y form is investigated.

2. Induced Representations

Consider a finite group G and its subgroup H . The whole symmetry group is decomposed into left cosets with respect to H :

$$G = \sum_{i=1}^n s_i H. \quad (1)$$

There are two physical cases in which this decomposition is of great use. The atoms in a symmetric nanostructure are

located at points with local symmetry H , which may coincide with the full group G , or with any of its subgroup, including a subgroup consisting of an identity element only. The action of the left coset representatives in (1) on initial atom results in an *orbit* of this atom. The second case is the band theory of solids [1, 2], where subgroup H is the wavevector group. The action of the left coset representatives s_i on the wavevector k results in a star $\{k\}$ of this vector. The number n of atoms, forming the orbit of an atom and the number n of prongs in a star of the wavevector, is given by the relation

$$n = \frac{|G|}{|H|}, \quad (2)$$

where the modulus sign stands for the number of elements of a group.

Consider IR D^k of subgroup H and its basis set $\{\varphi_\mu, \mu = 1, \dots, n_k\}$, where n_k stands for the dimension of D^k . According to the theorem on induced representation [1, 2], a set of functions $s_i \varphi_\mu$ ($i = 1 \dots n, \mu = 1, \dots, n_k$) is invariant in the group G and forms the basis of induced representation $D^k \uparrow G$, given by the formula

$$(D^k \uparrow G)(g)_{i\mu, j\nu} = D^k(s_i^{-1} g s_j)_{\mu\nu} \delta(s_i^{-1} g s_j, H), \quad (3)$$

where

$$\delta(s_i^{-1} g s_j, H) = \begin{cases} 1, & \text{if } s_i^{-1} g s_j \in H \\ 0, & \text{if } s_i^{-1} g s_j \notin H. \end{cases} \quad (4)$$

In a general case, the induced representation (3) is reducible in G and is decomposed into the sum of its IRs Γ^q of G as follows:

$$D^k \uparrow G = \sum_q f_q \Gamma^q, \quad (5)$$

where f_q stand for frequencies of appearance of IRs Γ^q . For the decomposition of induced representation (3), one can apply Frobenius reciprocity theorem [27], according to which the frequency f_q of IR Γ_q of the whole group in the decomposition of induced representation $D^k \uparrow G$ equals the frequency of appearance of IR D^k in the decomposition of IR Γ^q subduced to H :

$$f(\Gamma^q | D^k \uparrow G) = f(D^k | \Gamma^q \downarrow H). \quad (6)$$

Thus, according to Frobenius reciprocity theorem, the values of f_q in the right-hand side of (5) are given by the formula

$$f(\Gamma^q | D^k \uparrow G) = \frac{1}{|H|} \sum_{h \in H} \chi(D^k(h)) \chi^*(\Gamma^q(h)), \quad (7)$$

where χ stand for characters of representations.

3. Molecular Vibrations and SALCs

Consider normal vibration construction for symmetrical molecules. The displacements $\{x_1, y_1, z_1\}$ of an atom A_1 from

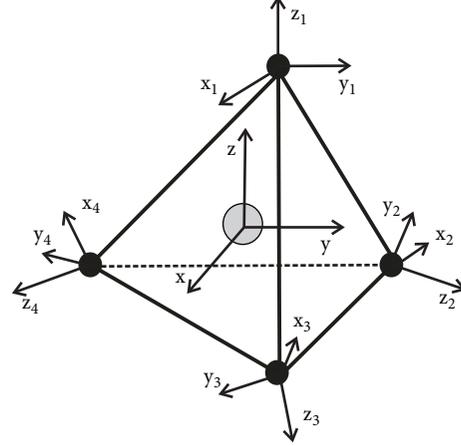


FIGURE 1: Basis set for vibrations in tetrahedral molecule. $x_i, y_i,$ and z_i are atomic displacements.

the equilibrium position are the components of the vector. Under the operations of the subgroup H , these coordinates are transformed by IRs D^k of this subgroup. The set of $3n$ displacements of n atoms forming an orbit of atom A_1 must be transformed by the representation (reducible) of the entire group G . The displacements of other atoms are obtained by the action of left coset representatives s_i (see formula (1)) on the basis set of the first atom. Let the atom A_1 be transformed into the atom A_i by the element s_i , and the same element transforms the basis $\{x_1, y_1, z_1\}$ into basis $\{x_i, y_i, z_i\}$. Then, under the action of the elements of the symmetry group of this atom, $H_i = s_i H s_i^{-1}$, the displacements $\{x_i, y_i, z_i\}$ are transformed by the conjugate representation $D_i^k(h_i) = D^k(s_i^{-1} h_i s_i)$ of this group. This means that under the action the whole symmetry group G basis set of displacements of an orbit is transformed as a basis of the induced representation $D^k \uparrow G$. Note that its matrix depends on the choice of left coset representatives, but its decomposition into IRs of G does not. To calculate the set of IRs in the decomposition of the whole matrix of displacements, one does not need to construct it. This decomposition can be done making use of the Frobenius reciprocity theorem (i.e., by summation of characters on the subgroup in formula (7)).

Consider CH_4 molecule of T_d symmetry. The basis set of atomic displacements is shown in Figure 1. The first atom H_1 is in z -axis and directions of the axis on it are the same as those on central atom. The basis sets on other atoms are obtained by C_2 rotations about corresponding axis. Local symmetry group of atom H_1 is C_{3v} . The stretching vibrations (z -component) of atom A_1 displacements belong to IR A_1 of C_{3v} and bending vibrations (x - and y -components) belong to IR E of C_{3v} . The decomposition of the induced representations can be easily done by Frobenius reciprocity theorem (7) and making use of characters of C_{3v} and of T_d on C_{3v} , presented in Table 1. Making use of formula (7), one obtains that $A_1 \uparrow T_d = A_1 + T_2$ and $E \uparrow T_d = E + T_1 + T_2$. To obtain all vibration modes, one should add vibrations of central atom, which belong to IR T_2 , and subtract the representation of

TABLE 1: Part of character table of group T_d on its subgroup C_{3v} (top part) and characters of IRs A_1 and E of group C_{3v} . (bottom part).

Group/subgroup	IR	Element (number in class)/character		
		$E(1)$	$C_3(2)$	$\sigma_v(3)$
T_d	A_1	1	1	1
	A_2	1	1	-1
	E	2	-1	0
	T_1	3	0	-1
	T_2	3	0	1
C_{3v}	A_1	1	1	1
	E	2	-1	0

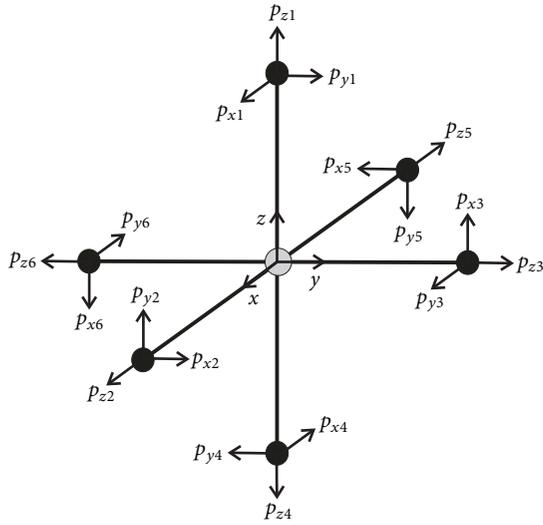


FIGURE 2: Basis set for SALC of atomic orbitals in octahedral molecule.

the whole molecule displacements T_2 and rotations T_1 (see [6]). Thus, one obtains total set of vibration modes of CH_4 molecule $A_1 + E + 2T_2$. Hence, it follows that as opposed to standard methods [4–6], where a multidimensional character of total vibration representation is constructed explicitly, the induced representation method makes it possible to obtain the same results by the character's analysis on local subgroup only.

The method of construction of SALCs of atomic wavefunctions in molecules is very similar to the above discussed technique. Consider p -orbitals in octahedral complex, in which six atoms are in coordinate directions (see Figure 2). Directions of the axis of the first atom in the six-atom orbit are the same as those of central atom. The axes of the second and third centers are obtained by counterclockwise rotation by 120° and 240° , respectively, about axis (III) and the rest of basis set is obtained by the space inversion. To convert basis functions on the centers 4, 5, and 6 into standard form, one can rename p_x and p_y basis functions, but it is not essential in our general consideration. Functions p_{z1} and $\{p_{x1}, p_{y1}\}$ belong to IRs A_1 and E , respectively, of local group

C_{4v} of the first atom. These orbitals are called σ - and π -orbitals, respectively. Under the action of the elements of O_h group, these functions are transformed independently by induced representations $A_1 \uparrow O_h$ and $E \uparrow O_h$, whose dimensions are 6 and 12, respectively. The characters of these induced representations are the same as those constructed for σ - and π -orbitals in O_h symmetry explicitly [7]. It follows from Frobenius reciprocity theorem that there is no need to construct these characters and it is sufficient to check the orthogonality of characters of IRs A_1 and E of group C_{4v} with characters of IRs of the whole group O_h . These characters are presented in Table 2. It is seen from Table 2 that the character of IR A_1 of C_{4v} group is not orthogonal to the characters of IRs A_{1g} , E_g , and T_{1u} of O_h . Thus, we obtain that $A_1 \uparrow O_h = A_{1g} + E_g + T_{1u}$. Similar analysis for IR E of C_{4v} results in the fact that π -orbitals belong to IRs T_{1g} , T_{1u} , T_{2g} , and T_{2u} . These sets of orbitals are the same as those obtained for σ - and π -orbitals, making use of explicit construction of six- and twelve-dimensional matrix [7]. We see that IR T_{1u} appears twice in the whole basis set constructed from p -orbitals of one orbit of atoms. These basis sets are labeled by physical quantum number (i.e., IR A_1 or E of local group C_{4v}). In the case when the atoms in symmetrical clusters are on the planes of symmetry, it is possible to distinguish basis sets of repeating IRs by the proper choice of intermediate group [22]. This technique is useful for Cooper pairs [23] and will be considered in the next section.

4. Additional Quantum Numbers for Induced Representations

When the atoms are on the planes of symmetry, SALCs contain repeating IRs [22]. To label repeating IRs, it is possible to use the transitivity property of induction, which means that the two ways of induction, from H directly into G and via an intermediate subgroup F , result in the same IRs:

$$D^k \uparrow G \propto (D^k \uparrow F) \uparrow G. \quad (8)$$

The decomposition of induced representation in the left-hand side of (8) into IRs of G is written as follows:

$$D^k \uparrow G = \sum_q f_q^k \Gamma^q. \quad (9)$$

Consider an alternative route of induction. After inducing into the intermediate subgroup F , we may decompose the result into IRs B^i of F :

$$D^k \uparrow F = \sum_i f_i^k B^i. \quad (10)$$

Similar decomposition is carried out after inducing each one of IRs B^i into G :

$$B^i \uparrow G = \sum_q f_q^i \Gamma^q. \quad (11)$$

According to the transitivity of induction theorem (8), the frequencies are connected by the relation

$$f_q^k = \sum_i f_i^k f_q^i. \quad (12)$$

TABLE 2: Characters of group O_h on its subgroup C_{4v} (top part, characters of u -IRs are shown in parenthesis, when they differ from g -IRs) and characters of IRs A_1 and E of group C_{4v} (bottom part).

Group/subgroup	IR	Element (number in class)/character				
		$E(1)$	$C_{2z}(1)$	$C_{4z}(2)$	$\sigma_v(2)$	$\sigma_v'(2)$
O_h	$A_{g(u)}$	1	1	1	1 (-1)	1 (-1)
	$A_{2g(u)}$	1	1	-1	1 (-1)	-1 (1)
	$E_{g(u)}$	2	2	0	2 (-2)	0
	$T_{1g(u)}$	3	-1	1	-1 (1)	-1 (1)
	$T_{2g(u)}$	3	-1	-1	-1 (1)	1 (-1)
C_{4v}	A_1	1	1	1	1	1
	E	2	-2	0	0	0

If frequencies in two-step induction in (10) and (11) do not exceed unity, every repeating IR in (9) acquires unique additional quantum number — index i of IR of intermediate subgroup. This technique will be used in the next sections for additional quantum numbers of Cooper pairs.

5. Space-Group Approach to the Wavefunction of a Cooper Pair

Following Ginzburg and Landau [28], we consider SOP (superconducting order parameter) to be identical with a Cooper pair wavefunction. Hereby, we can take advantage of general quantum mechanical rule for construction of two-electron state. Thus, the wavefunction of two-electron state is constructed as a direct (Kronecker) product of one-electron wavefunctions. If the electrons are equivalent, the requirement of antisymmetry of the total wavefunction makes partial reduction of the total two-electron space into singlet and triplet subspaces possible. Thus, making use of the Pauli exclusion principle, we obtain that spatial part of a singlet (triplet) pair belongs to symmetrized (antisymmetrized) Kronecker square of one-electron wavefunction. Irreducible representations of space groups are induced from wavevector group [1–3, 26] and are defined by formula (3). The method of the decomposition of Kronecker squares of induced representations of finite group into symmetrized and antisymmetrized parts was developed by Mackey [12] and applied to space groups by Bradley and Davies [13].

The structure of the Kronecker square of IRs of a space group depends on the structure of the space group G relative to wavevector group H . The double coset decomposition of \underline{G} relative to H is written as

$$G = \sum_{\delta} Hd_{\delta}H. \quad (13)$$

For each double coset representative in (13), the intersection subgroup is considered:

$$M_{\delta} = d_{\delta}Hd_{\delta}^{-1} \cap H. \quad (14)$$

The representation of group M_{δ} is defined by the following formula:

$$P_{\delta}^{k\pm}(m) = D^k(m) \times D^k(d_{\delta}^{-1}md_{\delta}), \quad (15)$$

where $m \in M_{\delta}$. For each self-inverse double coset (i.e., $Hd_{\delta}H = Hd_{\delta}^{-1}H$), there are two extensions of P_{δ}^k into extended intersection subgroup $M_{\delta}^* = M_{\delta} + d_{\delta}M_{\delta}$, whose characters are as follows:

$$\chi(P_{\delta}^{k+}(d_{\delta}m)) = \chi(D^k(d_{\delta}md_{\delta}m)) \quad (16)$$

$$\chi(P_{\delta}^{k-}(d_{\delta}m)) = -\chi(D^k(d_{\delta}md_{\delta}m)), \quad (17)$$

where $m \in M_{\delta}$. Then, the symmetrized and antisymmetrized parts of the Kronecker square of the IR of the space group are given by the two following formulae, respectively:

$$[(D^k \uparrow G) \times (D^k \uparrow G)] = [D^k \times D^k] \uparrow G + \sum_{\alpha} P_{\alpha}^{k+} \quad (18)$$

$$\uparrow G + \sum_{\alpha} P_{\alpha}^k \uparrow G$$

$$\{(D^k \uparrow G) \times (D^k \uparrow G)\} = \{D^k \times D^k\} \uparrow G + \sum_{\alpha} P_{\alpha}^{k-} \quad (19)$$

$$\uparrow G + \sum_{\alpha} P_{\alpha}^k \uparrow G.$$

The first items on the right-hand sides of (18) and (19) correspond to the double coset defined by the identity element. The summations in the second items in the right-hand side of (18) and (19) run over all self-inverse double cosets. The last summations in the right-hand side of (18) and (19) correspond to non-self-inverse double cosets (i.e., $Hd_{\beta}H \neq Hd_{\beta}^{-1}H$). According to the Pauli exclusion principle, the symmetrized Kronecker square (equation (18)) defines the spatial part of the singlet state (antisymmetrized with respect to spin coordinates) and the antisymmetrized Kronecker square (equation (19)) defines the spatial part of the triplet state, which is symmetrical with respect to spin coordinates. It follows from the Mackey-Bradley theorem that possible symmetries of singlet and triplet states are different for identity and self-inverse double cosets and are the same for non-self-inverse double cosets. Since total momentum of a Cooper pair equals zero, the following relation should be fulfilled for the k -vector and double coset representative:

$$\vec{k} + d_{\alpha}\vec{k} = \vec{b}, \quad (20)$$

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

It is clear from (20) that if k is inside the BZ, one can take the space inversion I or C_2 rotation about the axis normal to k . At the surface of a BZ where $\vec{k} = \vec{b}/2$, double coset defined by identity element also results in two-electron state with zero total momentum. Pairing of electrons with equal moments was proposed for pseudogap states in cuprate superconductors and was called Amperean pairing [29]. Thus double coset defined by identity element corresponds to Amperean pairing.

For k , a general point of a Brillouin zone relation (20) is fulfilled for double coset defined by the space inversion and group M_α^* consists of the identity element E and the space inversion I only. It is seen from formulas (15)-(17) that in this case symmetrized square belongs to even IR of group C_i and antisymmetrized square belongs to odd IR of C_i . The decomposition of corresponding induced representations can be easily done making use of Frobenius reciprocity theorem (formula (7)). Thus, one obtains that each even (odd) IR of the whole group appears in symmetrized (antisymmetrized) square with the frequency equal to its dimension.

The space-group approach is an alternative to phenomenological or point group approach [30–33] in which the pair function is expressed in terms of spherical functions, similar to spherical harmonics in crystal field theory [7]. In point group approach, spatial part of a singlet pair is even and spatial part of triplet pair is odd [16, 30, 31]. It can be easily shown that this relation is violated for two-dimensional small IRs on the lines of symmetry [14, 15, 21]. Indeed, it follows from formulas (15)-(17) that for two-dimensional small IRs $\chi[P_I^{k\pm}(E)] = 4$ and $\chi[P_I^{k\pm}(I)] = \pm 2$. Hence, it follows that neither P_I^{k+} is decomposed into even IRs only nor P_I^{k-} is decomposed into odd IRs only. It is also clear from formulas (15)-(17) than on lines of symmetry the set of possible IRs for a pair depends on the IR of one-electron state. The direct relation between multiplicity and parity is also violated for nonsymmorphic space groups on the surface of a BZ [14, 18–20].

It follows from the Blount theorem [32] that there are no symmetry requirements for lines of nodes in triplet case. Also phenomenological functions for D_{4h} group in a triplet case are nodeless [33]. It was pointed out [34–36] that a contradiction exists between experimental lines of nodes in Sr_2RuO_4 and nodeless model functions [33]. It will be shown in the next section that nodal and nodeless basis sets for two-dimensional IRs can be distinguished by additional quantum numbers.

6. Nodes on Symmetry Planes

In the symmetry plane, the group M_α^* of a pair is C_{2h} and it follows from formulas (15)-(17) that spatial part of a singlet pair belongs to IR A_g and that of triplet pair belongs to IR B_u of C_{2h} .

In L - S coupling scheme, total pair wavefunction is a direct product of its spatial and spin parts. Symmetrized Kronecker square of spatial part is multiplied by singlet spin function S^0 , which belongs to IR A_{1g} , and the nodal structure of a singlet pair is the same as that of its spatial part. The triplet spin

state consists of three components: S_0^1 , S_1^1 , and S_{-1}^1 , where the subscript denotes spin projection on z -axis. In the commonly accepted notation, \hat{z} stands for S_0^1 and \hat{x} and \hat{y} are linear combinations of S_1^1 and S_{-1}^1 . In the S_0^1 component, the spins of electron in a pair are opposite and this state is called OSP (opposite spin pairing). In the S_1^1 and S_{-1}^1 components, the electron spins in a pair are equal and these states (or their linear combinations \hat{x} and \hat{y}) are called ESP (equal spin pairing). In the case of D_{4h} symmetry, OSP spin belongs to IR A_{2g} and ESP total spin belongs to IR E_g . Theorem on the direct product of IR Γ and induced representation $D^k \uparrow G$ [1, 2] is written as

$$\Gamma \times (D^k \uparrow G) = [(\Gamma \downarrow H) \times D^k] \uparrow G. \quad (21)$$

Hence, it follows that the symmetry of OSP pair on the plane is $(A_{2g} \downarrow C_{2h}) \times B_u$ and the symmetry of ESP pair on the plane is $(E_g \downarrow C_{2h}) \times B_u$. These characters are also presented in Table 3. Since these IRs are induced into the whole group (see formulas (18) and (19)), the final results may be easily obtained making use of Frobenius reciprocity theorem. The absence of any IR of C_{2h} in the right column results in the absence of some IRs of the whole group for the k -vector on this plane. The intersection of symmetry plane with Fermi surface results in a line. Thus, the absence of any IR on the plane results in a symmetry-protected line of nodes. Some symmetry protected lines of nodes can be identified in a singlet case and for spatial part in a triplet case making use of Table 3 and Frobenius reciprocity theorem. It is seen from Table 3 that if in a triplet case both ESP and OSP pairs are taken into account, all odd IRs of C_{2h} , namely, A_u and B_u , are possible on the planes and there are no symmetry-protected lines of nodes. This conclusion is in agreement with Blount theorem, according to which in a triplet case, symmetry-protected lines of nodes are “vanishingly improbable” [32]. On the other hand, in axial symmetry, OSP and ESP pairs due to interaction with crystal field will have different energies and only one type of pairing, namely, ESP or OSP, will take place. In the case of Sr_2RuO_4 , it is assumed that pairing is of OSP type [34–36]. Hence, it follows from Table 3 that if only one type of pairing (ESP or OSP) takes place, symmetry-protected lines of nodes are possible.

In order to consider two-dimensional IRs E_g and E_u in more detail, their characters on symmetry groups of planes are also presented in Table 3. It is immediately verified from the data of Table 3 that in the basal plane (001) IR E_g is completely forbidden for singlet pairs and E_u appears twice for spatial part of triplet pair. Hence, it follows that on basal plane in a singlet case there is a symmetry-protected line of nodes of IR E_g . In vertical planes, IR E_u appears ones in a triplet case and IR E_g appears ones in a singlet case. Note that according to Mackey-Bradley theorem, at general point of a BZ two-dimensional, IRs appear twice in the decomposition of the complete basis set. Thus, on vertical planes, one two-dimensional IR E_u is permitted and the other IR E_u is forbidden. Hence, it follows that such lines of nodes are not symmetry protected in terms of IRs of the whole group. These lines of nodes can be classified in terms of IRs of an intermediate group, namely, symmetry group of the plane

TABLE 3: Characters for singlet and triplet pairs on symmetry planes in a BZ of the space group with point group D_{4h} (top part) and characters of IR E_u of D_{4h} on these two types of planes (bottom part).

Type of function		E	σ_h	I	C_2	IRs of C_{2h}
Singlet	Spatial part	1	1	1	1	A_g
Triplet	Spatial part	1	1	-1	-1	B_u
Triplet	OSP ^(a)	1	1	-1	-1	B_u
Triplet	ESP ^(a)	2	-2	-2	2	$2A_u$
Triplet	OSP ^(b)	1	-1	-1	1	A_u
Triplet	ESP ^(b)	2	0	-2	0	$A_u + B_u$
IR of D_{4h}						
	E_g ^(a)	2	2	2	2	
	E_u ^(a)	2	2	-2	-2	
	E_g ^(b)	2	0	2	0	
	E_u ^(b)	2	0	-2	0	

(a) Basal plane $C_2 = C_{2z}$

(b) Vertical coordinate plane $C_2 = C_{2y}$ and vertical diagonal plane $C_2 = C_{2xy}$.

C_{2h} . It follows from formulae (15) and (17) that the symmetry of spatial part of a triplet pair on the plane corresponds to B_u of group C_{2h} . It is immediately verified that when inducing A_u from C_{2h} into G , one obtains the set of IRs, which also includes E_u . Hence, it follows that in general point of a BZ, one can label two basis sets of IR E_u by IR of intermediate group C_{2h} . The basis set $E_u(B_u)$ is nodeless on the plane and the basis set $E_u(A_u)$ is nodal on the plane.

7. Nonsymmorphic Space Groups and Symmetry Lines

In the center of a BZ and in some points on its faces, space inversion belongs to the wavevector group H . In this case, the double coset defined by identity element results in zero total momentum of two-electron state. In the center of a BZ, the first items in right-hand side (18), (19) are calculated by standard methods [37] and one obtains even spatial part only for triplet and singlet pair.

Consider as an example point $M(b_1/2, b_2/2, 0)$ in a space group $P4/nmm (D_{4h}^7)$ of Fe-pnictide superconductors [38]. In these materials, there two sheets of Fermi surface: one near point Γ and one near point M [38, 39]. In point M , space inversion belongs to the wavevector group and two electrons with equal nonzero moments combine into a Cooper pair and its zero total momentum is due to translation periodicity of a crystal. Since IRs are projective at this BZ point of nonsymmorphic space group D_{4h}^7 , projective factors appear in standard formulas for symmetrization (antisymmetrization) [37] for finite group IRs:

$$[\chi^2(g)] = \frac{\chi^2(g) + \chi(g^2)\omega(g, g)}{2} \quad (22)$$

$$\{\chi^2(g)\} = \frac{\chi^2(g) - \chi(g^2)\omega(g, g)}{2}. \quad (23)$$

It is seen from the results, presented in Table 4, that in a singlet pairing case, two even and one odd IRs are possible

TABLE 4: Spatial parts of pairs in point $M(b_1/2, b_2/2, 0)$, space group $P4/nmm (D_{4h}^7)^{(*)}$.

	Small IRs [26]	Possible pair symmetry
Singlet	t_1, t_2	$A_{1g} + B_{2g} + B_{2u}$
pairs	t_3, t_4	$A_{1g} + B_{2g} + A_{2u}$
Triplet	t_1, t_2	A_{1u}
pairs	t_3, t_4	B_{1u}

(*) Note that H and central extension of G coincide. IRs of H are projective and are denoted according to [26].

for each one of four projective IRs of group D_{4h} . In a triplet case, only one odd IR is possible for each IR of wavevector group.

The space-group approach to the wavefunction of a Cooper pair can be generalized for strong spin-orbit coupling case [15]. In this case, possible pair functions belong to antisymmetrized squares of double-valued representations. For k , a general point of a BZ and on the planes of symmetry, where double-valued small IRs are one-dimensional, corepresentations of magnetic groups [1, 26] should be used [15]. Consider two planes (001) in a BZ of D_{6h}^4 group, namely, $k_z = 0$ plane and $k_z = b_3/2$ plane. In D_{6h}^4 group, space group elements σ_z and C_{2z} are connected with translation τ , which equals to a half of Bravais lattice translation t_3 . [26]. Double-valued IRs [26] are presented in Table 5. It should be noted that since there are two phase factors for $k_z = b_3/2$, namely, one due to nonsymmorphic structure of group and one due to the double-valued IRs of spin rotation, double valued IRs are real [26].

Consider modifications of formulae (15)-(17) due to nonsymmorphic structure of group. Multiplication rule for space-group elements is as follows [1, 2, 26]:

$$\{\alpha | \tau_\alpha\} \times \{\beta | \tau_\beta\} = \{\alpha\beta | \tau_\alpha + \alpha\tau_\beta\}, \quad (24)$$

where α stands for a point group element and τ_α for its nonprimitive translation. Making use of this rule, one obtains

TABLE 5: Double-valued IRs on the (001) planes of symmetry of BZ for space group D_{6h}^4 [26].

		E	σ_h
$k_z = 0$	p_1	1	i
	p_2	1	$-i$
$k_z = b_3/2$	p_1	1	1
	p_2	1	-1

TABLE 6: Characters of representation P_I^- for Cooper pairs on symmetry planes (001) in the case of strong spin-orbit coupling (space-group D_{6h}^4).

	E	σ_h	I	C_{2z}	Decomposition
$k_z = 0$	4	0	-2	2	$A_g + 2A_u + B_u$
$k_z = b_3/2$	4	-4	-2	-2	$B_g + 3A_u$

that the transformation by inversion results in point $k = b_3/2$ a phase factor $\exp(-ib_3/2, t_3)$ in formula (15) for σ_z :

$$\begin{aligned} \{I | 0\} \{\sigma_z | \tau\} \{I | 0\} &= \{C_{2z} | I\tau\} \{I | 0\} \\ &= \{\sigma_z | -\tau\} \{\sigma_z | \tau + t_3\}. \end{aligned} \quad (25)$$

Also, there is a phase factor in formulas (16) and (17) for C_{2z} , since

$$\{C_{2z} | \tau\} \{C_{2z} | \tau\} = \{E | 2\tau\} = \{E | t_3\}. \quad (26)$$

One more phase factor appears, since small representations are double-valued and total phase factor for $C_{2z} \times C_{2z}$ equals one. Possible IRs of Cooper pairs for these planes are presented in Table 6. For $k_z = 0$, only one even IR A_g and all odd IRs A_u and B_u of group C_{2h} are possible. Hence, it follows that not all even IRs of D_{6h} appear in induced representation $A_g \uparrow D_{6h}$. Since all odd IRs of C_{2h} are possible, all odd IRs of D_{6h} are also possible. Thus, in agreement with Blount theorem, there are no symmetry-protected lines of nodes for odd IRs. It is also seen from Table 6 that for $k_z = b_3/2$ only one odd IR A_u is possible and there are symmetry-protected lines of nodes of odd IRs. Similar results were obtained by Micklitz and Norman [18–20]

In direction μk_z in a BZ for D_{6h} group, the wavevector group is C_{6v} and there are three two-dimensional double-valued IRs [26]. On the BZ face in direction $1/2 b_1 + \mu b_3$, symmetry group is C_{3v} and there are two one-dimensional IRs and one two-dimensional double-valued IR. The results for these two symmetrical directions presented in Table 7 show that in highly symmetrical directions possible pair symmetries depend on the internal quantum number — label of IR of little group. Due to large number of rotational elements in group C_{6v} , there is an analogy between IRs of this group and angular momentum j_z and it was called j_z dependence [21]. Present results for p_3 in $1/2 b_1 + \mu b_3$ direction are the same as that for $j_z = 1/2$ [21]. IRs p_1 and p_2 are one-dimensional and one can construct antisymmetrized square of p_1 or p_2 separately. These two states are connected by time-reversal and form a corepresentation $D(p_1, p_2)$. Antisymmetrized square of $D(p_1, p_2)$ consists of the same IRs as the result [21] for $j_z = 3/2$.

TABLE 7: Possible IRs of pair in symmetry directions in BZ for D_{6h} group in strong spin-orbit coupling case.

K	Small IR [26]	IR of D_{6h}
μb_3	p_1 or p_2	$A_{1g} + A_{1u} + E_u$
	p_3	$A_{1g} + A_{1u} + B_{1u} + B_{2u}$
$1/2 b_1 + \mu b_3$	p_1 or p_2	$A_{1u} + B_{2u}$
	$D(p_1, p_2)^{(*)}$	$A_{1g} + B_{2g} + 2A_{1u} + A_{2u} + B_{1u} + 2B_{2u}$
	p_3	$A_{1g} + B_{2g} + A_{1u} + B_{2u} + E_{1u} + E_{2u}$

(*) Corepresentation.

8. Basis Functions

In a general point of a BZ, the wavevector group H consists of an identity element only and the expressions for spatial parts of singlet and triplet pairs which follow from Mackey-Bradley theorem [13] may be written as

$$\psi_1^s = \varphi_{k_1}(r_1) \varphi_{Ik_1}(r_2) + \varphi_{k_1}(r_2) \varphi_{Ik_1}(r_1) \quad (27)$$

$$\psi_{k_1}^t = \varphi_{k_1}(r_1) \varphi_{Ik_1}(r_2) - \varphi_{k_1}(r_2) \varphi_{Ik_1}(r_1), \quad (28)$$

where k_1 denotes a general point in a representation domain of a BZ [1]. All one-electron wavefunctions are obtained when k_1 runs over representation domain of a BZ and all $|\widehat{G}|$ elements of the central expansion \widehat{G} of the space group G act on one-electron wavefunction $\varphi_{k_1}(r)$ [1, 2, 26]. The results of action of these elements on k_1 form a star $\{k_1\}$ of the wavevector. Thus, the number of one-electron basis functions of Cooper pair for k_1 a general point of a BZ equals $|\widehat{G}|$. Pair functions may be constructed for all k_1 in the representation domain of a BZ making use of formulas (27) and (28). Since the space inversion is included in formulas (27) and (28), the number of elements in two-electron basis set of definite multiplicity reduces to $|\widehat{G}|/2$.

We take a space group with central extension D_{4h} (i.e., symmetry group of unconventional superconductor S_2RuO_4 [32–35]) as an example of application of the space-group technique for construction of pair's function. The basis set for k_1 a general point in a BZ of a space group with D_{4h} point group is shown in Figure 3. Notations in [26] are used for the cubic point group elements. This makes the direct use of group multiplication table possible [26]. In these notations, h_1 is an identity element, h_{14} , h_4 , and h_{15} are rotations at $\pi/2$, π , and $3\pi/2$ about the axis (001), h_{26} , h_{27} , h_{37} , and h_{40} are reflections on planes (100), (010), (-110), and (110), respectively. Notations in [26] for the remaining elements of D_{4h} group may be obtained by making use of the following multiplication rules for h_{25} (space inversion):

$$\begin{aligned} h_{25} \times h_i &= h_{i+24}, & \text{if } 1 < i < 24, \\ h_{25} \times h_i &= h_{i-24}, & \text{if } 25 < i < 48. \end{aligned} \quad (29)$$

The labels of group elements h_i are used as subscripts of basis functions in Figure 3; for example,

$$\psi_2^t = h_2 \psi_1^t = \varphi_2(r_1) \varphi_{26}(r_2) - \varphi_2(r_2) \varphi_{26}(r_1). \quad (30)$$

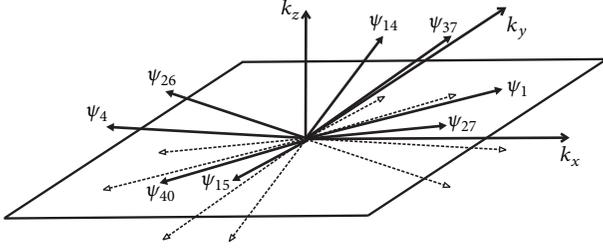


FIGURE 3: Basis set for Cooper in a general point of a BZ (D_{4h} symmetry). Basis function ψ_1 is defined by formula (28), where one-electron wavevector k_1 runs over basis domain of BZ and dashed lines correspond to wavevectors Ik_i . Basis function ψ_i is obtained by the action of point group element h_i on ψ_1 (notations in [26] are used; also see text).

TABLE 8: Spatial parts of triplet wavefunctions for IR E_u of D_{4h} group in x - y form ^(a). Basis function ψ_1 corresponds to arbitrary wave vector k_1 in a Brillouin zone in one-electron space and is built according to formula (28) (superscript t is dropped). Other basis functions are obtained by the action of half of the elements of group D_{4h} on ψ_1 (see Figure 3).

IR	Wavefunction	Nodes
E_u	$\psi_1 + \psi_{27} - \psi_4 - \psi_{26}$	No ^(b) (110) ^(c)
	$\psi_{14} + \psi_{37} - \psi_{15} - \psi_{40}$	No
$E_u^{A_{2g}}$	$\psi_1 - \psi_{27} - \psi_4 + \psi_{26}$	(010) (-110)
	$\psi_{14} - \psi_{37} - \psi_{15} + \psi_{40}$	(100)
$E_u^{B_{1g}}$	$\psi_1 + \psi_{27} - \psi_4 - \psi_{26}$	No (-110)
	$-\psi_{14} - \psi_{37} + \psi_{15} + \psi_{40}$	No
$E_u^{B_{2g}}$	$\psi_1 - \psi_{27} - \psi_4 + \psi_{26}$	(010) (110)
	$-\psi_{14} + \psi_{37} + \psi_{15} - \psi_{40}$	(100)

(a) Basis function for one-dimensional IRs and for E_u in chiral form are presented elsewhere [25].

(b) Nodes of the first type.

(c) Nodes of the second type.

In the case of induced representations, standard projection operator technique [37] may be reduced to the action of left coset representatives on the basis functions of subgroup [9] and one obtains the following formula for construction the wave function of a Cooper pair belonging to any IR Γ^q of \widehat{G} :

$$\Psi_i^{\Gamma^q} = \frac{|\Gamma^q|}{|\widehat{G}|} \sum_{h_k \in \widehat{G}} \Gamma_{ii}^q(h_k) h_k \psi_1. \quad (31)$$

The prime in (31) means that the sum includes only one of the two elements, connected by inversion.

Spatial parts of wavefunction of triplet Cooper pairs for IR E_u of D_{4h} group in x - y representation are presented in Table 8, where it is assumed that wavevector k_1 runs over basis domain of a BZ. The results for one-dimensional IRs and for E_u in chiral representation are presented elsewhere [25]. Nodal structure on the symmetry planes may be estimated as follows. Since pair function on the plane is invariant under plane reflection, the nodeless linear combination is unchanged under the action of the plane reflection. At the symmetry plane, mirror counterparts can merge or cancel. If

the signs of two mirror counterparts are changed under the action of plane reflection, they will cancel at the plane. The intersection of a nodal plane with Fermi surface results in symmetry-protected nodal line of SOP.

The action of reflection in (010) plane on the first line of E_u results in

$$h_{27}(\psi_1 + \psi_{27} - \psi_4 - \psi_{26}) = \psi_{27} + \psi_1 - \psi_{26} - \psi_4. \quad (32)$$

The sign is unchanged and there are no nodes in this plane. It is seen from Figure 3 that when k_1 runs over the basis domain of a BZ, the functions of the first line of E_u are around x -axis and the functions of the second line are around y -axis. Hence, we need to investigate nodes of the first function in plane (010) only and nodes of the second function in the plane (100) only. The action of reflection in (100) on the function of the second row results in

$$h_{26}(\psi_{14} + \psi_{37} - \psi_{15} - \psi_{40}) = \psi_{37} + \psi_{14} - \psi_{40} - \psi_{15}. \quad (33)$$

Hence, it follows that there are no nodes in plane (100) also. We will call the nodes due to cancelation of functions of one row as nodes of the first type.

In the case of two-dimensional IRs, there is one more possibility for lines of nodes, namely, cancelation between functions of the first and second rows. Reflection in plane (-110) h_{37} does not change the sign of the sum of two basis functions of E_u basis set:

$$\begin{aligned} h_{37}(\psi_1 + \psi_{27} - \psi_4 - \psi_{26} + \psi_{14} + \psi_{37} - \psi_{15} - \psi_{40}) \\ = \psi_{37} + \psi_{14} - \psi_{40} - \psi_{15} + \psi_{27} + \psi_1 - \psi_{26} - \psi_4. \end{aligned} \quad (34)$$

Thus, there are no nodes on plane (-110). The action of reflection in (110) plane h_{40} changes the sign of basis set:

$$\begin{aligned} h_{40}(\psi_1 + \psi_{27} - \psi_4 - \psi_{26} + \psi_{14} + \psi_{37} - \psi_{15} - \psi_{40}) \\ = \psi_{40} + \psi_{15} - \psi_{37} - \psi_{14} + \psi_{26} + \psi_4 - \psi_{27} - \psi_1. \end{aligned} \quad (35)$$

Hence, it follows that the basis set of IR E_u has a nodal plane (110). We will call the nodes, resulting from the cancelation of basis functions belonging to different rows of two-dimensional IR, nodes of the second type.

It is immediately verified that multiplication of E_u by all even one-dimensional IRs results also in E_u . Thus, the other E_u basis sets can be obtained by projection on IRs E_u transformed by A_{2g} , B_{1g} , and B_{2g} . Basis sets of E_u symmetry, labeled by these one-dimensional IRs, written as superscripts, are also presented in Table 8. These basis sets and the results of their nodal structure analysis are presented in Table 8. It is seen from Table 8 that basis sets $E_u^{A_{2g}}$ and $E_u^{B_{2g}}$ have nodes of the first type on two vertical coordinate planes, but basis sets E_u and $E_u^{B_{1g}}$ have no nodes of the first type. It is also seen from Table 8 that all IRs have one vertical nodal plane of the second type. Recall that it follows from Mackey-Bradley theorem that E_u appears twice in complete basis set, but once of each vertical plane (see Table 3 and discussions in the text). Consider E_u and $E_u^{A_{2g}}$, differing by nodal quantum number on the plane (100). It is seen from Table 8, that in

agreement with the results of Table 3, there is one nodeless IR, and the other is nodal on each vertical plane. The same result is valid for other pair of IRs $E_u^{B_{1g}}$ and $E_u^{B_{2g}}$. The authors of experimental works [34–36] on topological superconductor Sr_2RuO_4 obtained vertical lines of nodes of odd triplet SOP and concluded that OSP pairing is the most probable. In D_{4h} group, the symmetry of OSP spin is A_{2g} . Since we investigated products of E_u basis set by all one-dimensional IRs, our results include symmetry of OSP case and confirm that vertical lines of nodes are possible for OSP pairs of E_u symmetry. Note that there are two different forms of IR E_u , namely, real and complex. Real form, considered in present work, is usually used in quantum chemistry [7, 8]. Basis functions of complex form [26] have definite momentum projection on z -axis and are considered elsewhere [25].

9. Conclusion

The advantages of applications of induced representation method to symmetrical molecules and Cooper pairs in solids are reviewed and some results for pairing in topological superconductors are obtained. It is shown that induced representation method makes it possible to simplify standard methods for normal vibrations and SALCs construction (i.e., list of permitted IRs is obtained by the analysis of character tables on local subgroup only). The applications of Mackey-Bradley theorem in the case of nonsymmorphic space groups and projective representations are further investigated and examples of UPt_3 and Fe-pnictide superconductors are considered. Nodal structure E_u SOP for D_{4h} symmetry in x - y representation is obtained and its dependence upon the addition quantum numbers is envisaged. These nodal structures are in qualitative agreement with experimental data for topological superconductor Sr_2RuO_4 .

Data Availability

The references to the sources of the data are in the paper, and at present there are no other places where they are available.

Conflicts of Interest

The author declares that there are no conflicts of interest.

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