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Subgroups of Hypercubic Group and Many Electron States in Crystals

E. F. Kustov,[1] V. G. Yarzhemsky,[2,3] and V. I. Nefedov[2]

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The point subgroups of index 2 of hypercubic group and their irreducible representations are obtained. The elements of the hypercubic group are represented as rotation about two axis. Possible physical meaning of hypercubic group for electron states is investigated. The reduction relations for the representations of orthogonal group O_4 on hypercubic group are obtained. These relations are used for additional classification of electron states in crystals.

KEY WORDS: many-electron systems; group theory; crystal symmetry; hypercubic group; quantum numbers.

1. INTRODUCTION

The four dimensional cubic group (hypercubic group), which is a subgroup of four dimensional unitary group U_4, and of four- dimensional rotational group O_4 (Cornwell, 1984) is applied in nuclear lattice theories (Kogut, 1979; Wilson, 1974). The single-valued and double-valued irreducible representations (IRs) of hypercubic group were obtained in Birman and Chen, (1971); Baake *et al.*, (1982); Mandula *et al.*, (1983); Mandula and Shpiz, (1984); Dai and Song, 2001. Four-dimensional Bravais lattices and space-groups were obtained in Mackay and Pawley, (1963); Neubuster *et al.*, (1971); Florek and Lulek, (1993). Transformation properties of momentum operators on hypercubic groups were investigated in Gockeler *et al.* (1996).

The four-dimensional cubic group is intermediate in the reduction of groups U_4 and O_4 on crystallographic point groups and can be applied for additional classification of many-electron states in crystals. The important property of 4-groups is that they conserve the four-dimensional properties of 4-vectors.

[1] Moscow Power Energy Institute; e-mail: kustovyf@mail.ru.
[2] Institute of General and Inorganic Chemistry of RAS, 31 Leninsky, 119991 Moscow, Russia.
[3] To whom correspondence should be addressed at; e-mail: vgyar@igic.ras.ru

The four-dimensional point groups were also applied for the classification of electron states in crystals (Kuzhukeev and Kustov, 1986; Kustov *et al.*, 2005). The symmetry groups of four-dimensional space, splitting into rotational groups R_3 and R_1, are very useful due to their isomorphism to discrete subgroups of Lorenz group (Below *et al.*, 1971) in physical applications. Also they can be considered as groups of discrete space-time coordinates (Lorente, 1986).

For physical applications the reduction schemes from the four-dimensional rotation group to hypercubic group and from hypercubic group to its subgroups are required. But systematic data on this subject are still absent and it is the main aim of the present work. Since we are interested in four-dimensional extensions of other crystallographic point groups we use the crystallographic notations with additional superscript 4. In this notations the hypercubic group is written as O_h^4 and its point subgroups of index 2 as T_d^4, T_h^4, O_4.

In the present work the elements of hypercubic group O_h^4 are expressed in terms of rotations around two different axes. Making use of these relations the reduction schemes of IRs of four-dimensional orthogonal group O_4 on the hypercubic group O_h^4 and its subgroups T_d^4, T_h^4, O^4 are obtained. We present also reduction relations from O_h^4 to the group $O_h^\theta = O_h + \theta O_h$ (where θ is time-inversion). Finally we show that classification of many-electron states in solids result in additional quantum number - the index of IR of group O_h^4.

2. THE SYMMETRY GROUP OF FOUR-DIMENSIONAL CUBE O_h^4

The group O_h^4 includes permutations of four coordinate axes, i.e. group P_4, consisting of 24 elements and inversions of each of four axes, i.e. group $P_2\times P_2\times P_2\times P_2$, where P_2 is the permutation group, consisting of 16 elements. Thus the total number of elements in group O_h^4 is equals to 384.

The group O_h^4 may be represented as left coset decomposition with respect to three dimensional cubic group O_h. Taking the inversion of fourth coordinate and permutations $P_{i,4}$ of the forth axis with spatial coordinates $(1, 2, 3) = (x, y, z)$ as a left coset representatives, we can write:

$$O_h^4 = O_h + \sum_{i=1}^{3} P_{i,4} O_h + I_4 \left(O_h + \sum_{i=1}^{3} P_{i,4} O_h \right) \qquad (1)$$

Connecting the fourth axis with some physical properties one obtains different physical applications of the four-dimensional cubic group. For instance, if the quantization axis of triplet two-electron state is the fourth coordinate, the elements $P_{i,4}O_h$ correspond to rotations in which the spin direction is transformed as the i-axis and the elements of O_h correspond to the case of fixed spins.

Let us consider four subgroups of O_h^4, which we denote by superscripts $(\alpha\beta\gamma)$. The group $O_h^{(\alpha\beta\gamma)}$ is a direct product of four inversions, which are isomorphic to permutation groups P_2 and permutation of three of the four coordinate axes $P_3^{(\alpha\beta\gamma)}$:

$$O_h^{(\alpha\beta\gamma)} = P_2 \times P_2 \times P_2 \times P_3^{(\alpha\beta\gamma)} \tag{2}$$

The permutations P_3 may be applied to one of the following set of coordinate axes, i.e. $(\alpha\beta\gamma) = (123), (124), (143), (423)$. In the case of $(\alpha\beta\gamma) = (123)$ one can consider the fourth axis as a time. Thus the group $O_h^{(123)}$, which we denote as O_h^{θ} ,is equal to $O_h + \theta O_h$. It is the grey Shubnikov group, i.e. covering group for all Shubnikov groups of cubic symmetry. Also the fourth axis may be considered as axis of any property, say the quantization axis of spin. For example, the group $O_h^{(124)}$ corresponds to the structure with the spatial symmetry D_{4h} with the four fold axis in z-direction. Under the action of elements of this group the spin is permuted with the four axial directions of the plane (x, y).

3. POINT SUBGROUPS OF O_h^4

The elements and characters of the O_h^4 group are presented in Table I. The relation between between present notations (see also Kustov *et al.*, 2005) and that of Baake *et al.*, (1982) is also shown in Table I. Since the characters of IRs of group O_h^4 are known (Birman and Chen, 1971; Baake *et al.*, 1982; Mandula *et al.*, 1983; Mandula and Shpiz, 1984; Dai and Song, 2001; Neubuster *et al.*, 1971; Florek and Lulek, 1993; Kuzhukeev and Kustov, 1986; Kustov *et al.*, 2005), its subgroups can be easily identified with those group elements whose characters for nontrivial one-dimensional IRs equal to unity. Thus we have three subgroups of O_h^4 which are T_h^4, T_d^4 and O^4, and T^4 which is subgroup of T_h^4 i.e. point subgroups of O_h extended by permutation of the fourth axis with spatial coordinate axes. The characters of single-valued IRs for groups O^4, T_d^4, $T_h^4$and T^4 are presented in Tables II, III, IV and V respectively. The reduction schemes for the IRs O_h^4 onto its subgroups are presented in Table VI. A complete reduction scheme from group U_4 via four-dimensional orthogonal group O_4 and Lorenz group L is shown in Fig. 1. Going over to the group O_h^{θ} (grey Shubnikov group $O_h + \theta O_h$) it should be noted that there are two possibilities for representations of Shubnikov groups (Bradley and Cracknell, 1972). In the first approach one can consider Shubnikov groups in the abstract sense and construct their characters by using of multiplication rules. The second approach is based on the special feature of θ as time-reversal. In the present work we apply the first approach only. Thus there are two extensions for the elements of left coset θO_h i.e. $\chi(\theta g) = \pm\chi(g)$.These extensions are marked by corresponding superscripts in Table VI. IR of O_h^4 group are labelled according to Kustov *et al.*, (2005).

Table I. Characters X_i of IRs and the Numbers n_i of Classes c_i of Group O_h^4

		c_1	c_9	c_5	c_3	c_{15}	c_7	c_8	c_{10}	c_{17}	c_{20}	c_6	c_4	c_2	c_{11}	c_{14}	c_{19}	c_{18}	c_{13}	c_{12}	c_{16}
[14]	[5]	1	4	6	12	12	4	24	24	32	32	1	12	12	12	24	32	32	12	48	48
X_1	$\chi_1^{(1)}$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
X_2	$\chi_3^{(1)}$	1	1	1	–1	–1	1	–1	–1	1	1	1	–1	1	–1	1	1	1	1	–1	–1
X_3	$\chi_2^{(1)}$	1	–1	1	1	–1	–1	–1	1	1	–1	1	1	1	–1	–1	–1	1	1	1	–1
X_4	$\chi_4^{(1)}$	1	–1	1	–1	1	–1	1	–1	1	–1	1	–1	1	1	–1	–1	1	1	–1	1
X_5	$\chi_1^{(2)}$	2	2	2	0	0	2	0	0	–1	–1	2	0	2	0	2	–1	–1	2	0	0
X_6	$\chi_2^{(2)}$	2	–2	2	0	0	–2	0	0	–1	1	2	0	2	0	–2	1	–1	2	0	0
X_7	$\chi_1^{(3)}$	3	3	3	1	1	3	1	1	0	0	3	1	–1	1	–1	0	0	–1	–1	–1
X_8	$\chi_3^{(3)}$	3	3	3	–1	–1	3	–1	–1	0	0	3	–1	–1	–1	–1	0	0	–1	1	1
X_9	$\chi_2^{(3)}$	3	–3	3	1	–1	–3	–1	1	0	0	3	1	–1	–1	1	0	0	–1	–1	1
X_{10}	$\chi_4^{(3)}$	3	–3	3	–1	1	–3	1	–1	0	0	3	–1	–1	1	1	0	0	–1	1	–1
X_{11}	$\chi_1^{(4)}$	4	2	0	2	2	–2	0	0	1	1	–4	–2	0	–2	0	–1	–1	0	0	0
X_{12}	$\chi_3^{(4)}$	4	2	0	–2	–2	–2	0	0	1	1	–4	2	0	2	0	–1	–1	0	0	0
X_{13}	$\chi_2^{(4)}$	4	–2	0	2	–2	2	0	0	1	–1	–4	–2	0	2	0	1	–1	0	0	0
X_{14}	$\chi_4^{(4)}$	4	–2	0	–2	2	2	0	0	1	–1	–4	2	0	–2	0	1	–1	0	0	0
X_{15}	$\chi_1^{(6)}$	6	0	–2	0	2	0	–2	0	0	0	6	0	–2	2	0	0	0	2	0	0
X_{16}	$\chi_2^{(6)}$	6	0	–2	0	–2	0	2	0	0	0	6	0	–2	–2	0	0	0	2	0	0
X_{17}	$\chi_4^{(6)}$	6	0	–2	–2	0	0	0	2	0	0	6	–2	2	0	0	0	0	–2	0	0
X_{18}	$\chi_3^{(6)}$	6	0	–2	2	0	0	0	–2	0	0	6	2	2	0	0	0	0	–2	0	0
X_{19}	$\chi_1^{(8)}$	8	4	0	0	0	–4	0	0	–1	–1	–8	0	0	0	0	1	1	0	0	0
X_{20}	$\chi_2^{(8)}$	8	–4	0	0	0	4	0	0	–1	1	–8	0	0	0	0	–1	1	0	0	0

Table II. IRs of Subgroup T_h^4 Defined by IR X_2 of the Group O_h^4 and Numbers of Elements in Classes. The Classes are Denoted According to O_h^4 Group

O_h^4	c_1	c_9	c_5	c_7	c_{17}	c_{17}	c_{20}	c_{20}	c_6	c_2	c_{14}	c_{19}	c_{19}	c_{18}	c_{18}	c_{13}
T_h^4	1	4	6	4	16	16	16	16	1	12	24	16	16	16	16	12
X_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
X_2	1	−1	1	−1	1	1	−1	−1	1	1	−1	−1	−1	1	1	1
X_3'	1	1	1	1	ϵ	ϵ^2	ϵ	ϵ^2	1	1	1	ϵ	ϵ^2	ϵ	ϵ^2	1
X_3''	1	1	1	1	ϵ^2	ϵ	ϵ^2	ϵ	1	1	1	ϵ^2	ϵ	ϵ^2	ϵ	1
X_4'	1	−1	1	−1	ϵ	ϵ^2	$-\epsilon$	$-\epsilon^2$	1	1	−1	$-\epsilon$	$-\epsilon^2$	ϵ	ϵ^2	1
X_4''	1	−1	1	−1	ϵ^2	ϵ	$-\epsilon^2$	$-\epsilon$	1	1	−1	$-\epsilon^2$	$-\epsilon$	ϵ^2	ϵ	1
X_5	3	3	3	3	0	0	0	0	3	−1	−1	0	0	0	0	−1
X_6	3	−3	3	−3	0	0	0	0	3	−1	1	0	0	0	0	−1
X_7	4	2	0	−2	1	1	1	1	−4	0	0	−1	−1	−1	−1	0
X_8	4	−2	0	2	1	1	−1	−1	−4	0	0	1	1	−1	−1	0
X_9	6	0	−2	0	0	0	0	0	6	−2	0	0	0	0	0	2
X_{10}	6	0	−2	0	0	0	0	0	6	2	0	0	0	0	0	−2
X_{11}'	4	2	0	−2	ϵ^2	ϵ	ϵ^2	ϵ	−4	0	0	$-\epsilon^2$	$-\epsilon$	$-\epsilon^2$	$-\epsilon$	0
X_{11}''	4	2	0	−2	ϵ	ϵ^2	ϵ	ϵ^2	−4	0	0	$-\epsilon$	$-\epsilon^2$	$-\epsilon$	$-\epsilon^2$	0
X_{12}'	4	−2	0	2	ϵ^2	ϵ	$-\epsilon^2$	$-\epsilon$	−4	0	0	ϵ^2	ϵ	$-\epsilon^2$	$-\epsilon$	0
X_{12}''	4	−2	0	2	ϵ	ϵ^2	$-\epsilon$	$-\epsilon^2$	−4	0	0	ϵ	ϵ^2	$-\epsilon$	$-\epsilon^2$	0

$\epsilon = \exp(2\pi i/3)$.

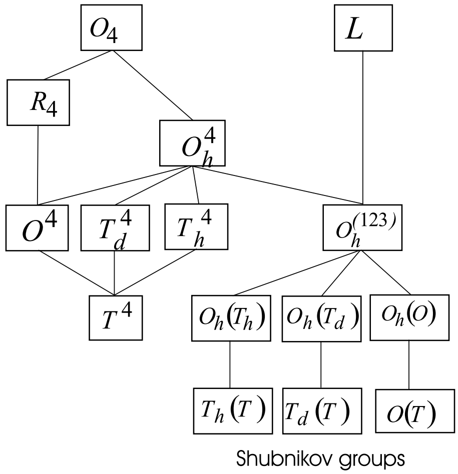

Fig. 1. Reduction scheme from continuous groups O_4, R_4 and L to four-dimensional point groups (denoted by superscript 4) and to point Shubnikov groups (unitary subgroups are written in brackets). For notation $O_h^{(123)}$ see text.

Table III. IRs of Subgroup T_d^4 Defined by IR X_3 of the Group O_h^4 and Numbers of Elements in Classes. The Classes are Denoted According to O_h^4 Group

O_h^4	c_1	c_3	c_5	c_{10}	c_{17}	c_{12}		c_{13}		c_4	c_{18}	c_2	c_6
T_d^4	1	12	6	24	32	24	24	6	6	12	32	12	1
X_1	1	1	1	1	1	1	1	1	1	1	1	1	1
X_2	1	−1	1	−1	1	−1	−1	1	1	−1	1	1	1
X_3	2	0	2	0	−1	0	0	2	2	0	−1	2	2
X_4	3	1	3	1	0	−1	−1	−1	−1	1	0	−1	3
X_5	3	−1	3	−1	0	1	1	−1	−1	−1	0	−1	3
X_6	3	1	−1	−1	0	1	−1	−3	1	1	0	1	3
X_7	3	1	−1	−1	0	−1	1	1	−3	1	0	1	3
X_8	3	−1	−1	1	0	−1	1	−3	1	−1	0	1	3
X_9	3	−1	−1	1	0	1	−1	1	−3	−1	0	1	3
X_{10}	4	2	0	0	1	0	0	0	0	−2	−1	0	−4
X_{11}	4	−2	0	0	1	0	0	0	0	2	−1	0	−4
X_{12}	6	0	−2	0	0	0	0	2	2	0	0	−2	6
X_{13}	8	0	0	0	−1	0	0	0	0	0	1	0	−8

Table IV. IRs of Subgroup O^4 Defined by IR X_4 of the Group O_h^4 and Numbers of Elements in Classes. The Classes are Denoted According to O_h^4 Group

O_h^4	c_1	c_{15}	c_5	c_8	c_{17}	c_{16}		c_{13}		c_{11}	c_{18}	c_2	c_6
O^4	1	12	6	24	32	24	24	6	6	12	32	12	1
X_1	1	1	1	1	1	1	1	1	1	1	1	1	1
X_2	1	−1	1	−1	1	−1	−1	1	1	−1	1	1	1
X_3	2	0	2	0	−1	0	0	2	2	0	−1	2	2
X_4	3	1	3	1	0	−1	−1	−1	−1	1	0	−1	3
X_5	3	−1	3	−1	0	1	1	−1	−1	−1	0	−1	3
X_6	3	1	−1	−1	0	1	−1	3	−1	1	0	−1	3
X_7	3	1	−1	−1	0	−1	1	−1	3	1	0	−1	3
X_8	3	−1	−1	1	0	−1	1	3	−1	−1	0	−1	3
X_9	3	−1	−1	1	0	1	−1	−1	3	−1	0	−1	3
X_{10}	4	2	0	0	1	0	0	0	0	−2	−1	0	−4
X_{11}	4	−2	0	0	1	0	0	0	0	2	−1	0	−4
X_{12}	6	0	−2	0	0	0	0	−2	−2	0	0	2	6
X_{13}	8	0	0	0	−1	0	0	0	0	0	1	0	−8

4. GEOMETRICAL REPRESENTATION OF O_h^4.

It follows from the theory of two-parametric groups (Petrashen and Trifonov, 1967), that each element of group R_4 may be represented as a product of two rotations about two axes of a direct product group $R_3 \times R_3$.

Table V. IRs of Subgroup T^4 Defined by IR X_2 of the Group T_h^4 and Numbers of Elements in Classes. The Classes are Denoted According to O_h^4 Group

O_h^4	c_1	c_6	c_2		c_5	c_{13}		c_{17}		c_{18}	
T^4	1	1	6	6	6	6	6	16	16	16	16
X_1	1	1	1	1	1	1	1	1	1	1	1
X_2	1	1	1	1	1	1	1	ϵ	ϵ^2	ϵ	ϵ^2
X_3	1	1	1	1	1	1	1	ϵ^2	ϵ	ϵ^2	ϵ
X_4	3	3	−1	−1	3	−1	−1	0	0	0	0
X_5	3	3	−1	−1	−1	3	−1	0	0	0	0
X_6	3	3	−1	−1	−1	−1	3	0	0	0	0
X_7	3	3	3	−1	−1	−1	−1	0	0	0	0
X_8	3	3	−1	3	−1	−1	−1	0	0	0	0
X_9	4	−4	0	0	0	0	0	1	1	−1	−1
X_{10}	4	−4	0	0	0	0	0	ϵ^2	ϵ	$-\epsilon^2$	$-\epsilon$
X_{11}	4	−4	0	0	0	0	0	ϵ	ϵ^2	$-\epsilon$	$-\epsilon^2$

$\epsilon = \exp(2\pi i/3)$

Table VI. Reduction Relations for Subgroups of O_h^4

O_h^4	O^4	T_d^4	T_h^4	T^4	$O_h^\theta, \theta = (123)$
X_1	X_1	X_1	X_1	X_1	A_{1g}^+
X_2	X_2	X_2	X_1	X_1	A_{2g}^+
X_3	X_2	X_1	X_2	X_1	A_{2u}^-
X_4	X_1	X_2	X_2	X_1	A_{1u}^-
X_5	X_3	X_3	X_3	X_2	E_g^+
X_6	X_3	X_3	X_4	X_2	E_u^-
X_7	X_4	X_4	X_5	X_3	$A_{1g}^+ + E_g^+$
X_8	X_5	X_5	X_5	X_3	$A_{2g}^+ + E_g^+$
X_9	X_5	X_4	X_6	X_3	$A_{2u}^- + E_u^-$
X_{10}	X_4	X_5	X_6	X_3	$A_{1u}^- + E_u^-$
X_{11}	X_{10}	X_{10}	X_7	X_8	$A_{1g}^+ + T_{1u}^+$
X_{12}	X_{11}	X_{11}	X_7	X_8	$A_{2g}^- + T_{2u}^+$
X_{13}	X_{11}	X_{10}	X_8	X_8	$A_{2u}^+ + T_{2g}^-$
X_{14}	X_{10}	X_{11}	X_8	X_8	$A_{1u}^+ + T_{1g}^-$
X_{15}	$X_6 + X_7$	X_{12}	X_9	$X_4 + X_5$	$T_{1g}^+ + T_{1u}^-$
X_{16}	$X_8 + X_9$	X_{12}	X_9	$X_4 + X_5$	$T_{2g}^+ + T_{2u}^-$
X_{17}	X_{12}	$X_8 + X_9$	X_{10}	$X_6 + X_7$	$T_{1g}^+ + T_{2u}^-$
X_{18}	X_{12}	$X_6 + X_7$	X_{10}	$X_6 + X_7$	$T_{2g}^+ + T_{1u}^-$
X_{19}	X_{13}	X_{13}	$X'_{11} + X''_{11}$	X_9	$E_g^- + T_{1u}^+ + T_{2u}^+$
X_{20}	X_{13}	X_{13}	$X'_{12} + X''_{12}$	X_9	$E_u^+ + T_{2g}^- + T_{1g}^-$

Thus each rotation of hypercube is represented as two rotations by angles ϕ_1 and ϕ_2 about two axes and the character of any IR $[j_1, j_2]$ of four-dimensional orthogonal group may be calculated as a product of two characters of R_3.

$$\chi^{[j_1,j_2]}(\phi_1,\phi_2) = \frac{\sin\frac{j_1+j_2+1}{2}\phi_1}{\sin\frac{\phi_1}{2}} \cdot \frac{\sin\frac{j_1-j_2+1}{2}\phi_2}{\sin\frac{\phi_2}{2}} \tag{3}$$

The rotation angles for hypercubic group were determined as follows. It is immediately verified that two IRs of O_4: vector representation {10} (curly brackets correspond to Young tables) and representation of antisymmetric tensor {11} are irreducible in the subduction to O_h^4 and are equivalent to X_{11} and X_{15} respectively. Hence it follows that the characters of these IRs are written in terms of rotational angles as follows:

$$\chi(X_{11}) = 4\cos\frac{\phi_1}{2}\cos\frac{\phi_2}{2} \quad (4)$$

$$\chi(X_{15}) = 4\left(\cos^2\frac{\phi_1}{2} + \cos^2\frac{\phi_2}{2}\right) - 2 \quad (5)$$

Hence for each of pure rotation element of O_h^4 we have a system of two equation for the determination of two angles. The resultant angles only for the proper rotations are presented in Table VI.

The other elements of O_h^4 are obtained multiplying by one-dimensional and three-dimensional inversions, since two-dimensional and four dimensional inversions are proper rotation.

5. ATOMIC STATES IN CRYSTALS

The covering group for O_h^4 is the four-dimensional unitary group, U_4, which is connected with the direct product of two orthogonal groups $O_3 \otimes O_3$ in three dimensions. That is why the IRs of U_4 are labelled by a pair of orbitals quantum numbers $[j_1, j_2]$ (Cornwell, 1984). Since the group O_3 is isomorphic to SU_2, the group U_4 has the subgroup of the direct product $O_3 \otimes SU_2$. Hence, it follows that any many-electron state with total orbital momentum L and total spin S belongs to IR $\Gamma^{[L,S]} = D^L \otimes D^S$ of group $O_3 \otimes O_3$. When this symmetry is reduced to O_3 this representation is reduced as:

$$\Gamma^{[L,S]} = \sum_j D^J, \quad J = L+S, L+S-1, L-S \quad (6)$$

In crystal field these states, characterized by total momentum J are further reduced. Since the total number of IRs of point groups is rather scant, the same IRs of point group appear in the decomposition of states with the same J. Hence it follows that additional quantum numbers required. The intermediate reduction from the unitary group U_4 to the hypercubic group makes possible to introduce addition quantum numbers. This reduction scheme is written as (Kustov, 1975a, 1975b, 1977, 1979):

$$O_4 \supset R_4 \rightarrow R_3 \times R_3 \supset O_h^4 \supset O \quad (7)$$

In the first step of reduction every IR of group O_4 splits into two as follows

Table VII. Classes of Group O_h^4 and Representation of its Proper Rotational Elements in Terms of Rotation Aroun Two Axis

Class	P_8	P_4	Number	rotations
C_1	$\{1^8\}$	$\{1^4\}$	1	(E, E)
C_2	$\{2^4\}$	$\{2^2\}$	12	(C_2, C_2)
C_3	$\{1^4 2^2\}$	$\{1^2 2\}$	12	
C_4	$\{2^4\}$	$\{1^2 2\}$	12	
C_5	$\{1^4 2^2\}$	$\{1^4\}$	6	(E, C_2)
C_6	$\{2^4\}$	$\{1^4\}$	1	
C_7	$\{1^2 2^3\}$	$\{1^4\}$	4	
C_8	$\{1^2 2^3\}$	$\{1^2 2\}$	24	(C_2, C_2)
C_9	$\{1^6 2\}$	$\{1^4\}$	4	
C_{10}	$\{1^2 24\}$	$\{1^2 2\}$	24	
C_{11}	$\{2^2 4\}$	$\{1^2 2\}$	12	(C_4^k, C_4^{-k}) , $k = 1, 3$
C_{12}	$\{4^2\}$	$\{4\}$	48	
C_{13}	$\{4^2\}$	$\{2^2\}$	12	(C_2, E_2)
C_{14}	$\{2^2 4\}$	$\{2^2\}$	24	
C_{15}	$\{1^4 4\}$	$\{1^2 2\}$	12	(C_4^k, C_4^k), $k = 2$
C_{16}	$\{8\}$	$\{4\}$	48	$(C_2, C_4^k,)$
C_{17}	$\{1^2 3^2\}$	$\{13\}$	32	(C_3^k, C_3^k)
C_{18}	$\{26\}$	$\{13\}$	32	(C_3^k, C_3^{-k})
C_{19}	$\{23^2\}$	$\{13\}$	32	
C_{20}	$\{1^2 6\}$	$\{13\}$	32	

(Littlwood, 1948; Wybourne, 1973):

$$[j_1, j_2] \rightarrow [j_1, j_2] + [j_1, -j_2] \tag{8}$$

The second step of reduction results in two following replacements:

$$[j_1, j_2] \rightarrow \left[\frac{j_1 + j_2}{2}\right] \times \left[\frac{j_1 - j_2}{2}\right] \tag{9}$$

$$[j_1, -j_2] \rightarrow \left[\frac{j_1 - j_2}{2}\right] \times \left[\frac{j_1 + j_2}{2}\right] \tag{10}$$

The character of IRs of group O_4 for the pure rotations of O_h^4 are easily obtained making use of formula (3). To obtain the characters for rotations with inversion, the character of the pure rotational element is multiplied by -1. The character of conjugate representation differs for the rotations with inversion, i.e.

Table VIII. Reduction of the IRs of Group O_4 in Subduction From O_4 to O_h^4

O_4	O_h^4
[0]	X_1
[0*]	X_4
[1]	X_{11}
[1*]	X_{14}
[11]	X_{15}
[2]	$X_7 + X_{18}$
[2*]	$X_{10} + X_{17}$
[21]	$X_{19} + X_{20}$
[22]	$X_5 + X_6 + X_{16}$
[3]	$X_{11} + X_{13} + X_{19}$
[3*]	$X_{12} + X_{14} + X_{20}$
[31]	$X_8 + X_9 + X_{15} + X_{16} + X_{17} + X_{18}$
[32]	$X_{12} + X_{13} + X_{19} + X_{20}$
[33]	$X_2 + X_3 + X_{15} + X_{16}$
[4]	$X_1 + X_3 + X_5 + X_7 + X_{15} + X_{16} + X_{18}$
[4*]	$X_2 + X_4 + X_6 + X_{10} + X_{15} + X_{16} + X_{17}$
[41]	$X_{11} + X_{12} + X_{13} + X_{14} + 2X_{19} + 2X_{20}$
[42]	$X_7 + X_8 + X_9 + X_{10} + X_{16} + 2X_{17} + 2X_{18}$
[43]	$X_{11} + X_{12} + X_{13} + X_{14} + X_{19} + X_{20}$
[44]	$X_1 + X_4 + X_5 + X_6 + X_{15} + X_{16}$
[5]	$2X_{11} + X_{13} + 2X_{19} + X_{20}$
[5*]	$X_{12} + 2X_{14} + X_{19} + 2X_{20}$
[51]	$X_5 + X_6 + X_7 + X_8 + X_9 + X_{10} + 3X_{15} + 2X_{16} + 2X_{17} + 2X_{18}$
[52]	$X_{11} + X_{12} + X_{13} + X_{14} + 3X_{19} + 3X_{20}$
[53]	$X_7 + X_8 + X_9 + X_{10} + 2X_{15} + X_{16} + 2X_{17} + 2X_{18}$
[54]	$X_{11} + X_{14} + 2X_{19} + 2X_{20}$
[55]	$X_5 + X_6 + 2X_{15} + X_{16}$
[6]	$X_1 + 2X_7 + X_8 + X_9 + X_{15} + X_{16} + X_{17} + 3X_{18}$
[6*]	$X_4 + X_8 + X_9 + 2X_{10} + X_{15} + X_{16} + 3X_{17} + X_{18}$
[61]	$2X_{11} + 2X_{12} + 2X_{13} + 2X_{14} + 4X_{19} + 4X_{20}$
[62]	$X_1 + X_2 + X_3 + X_4 + 2X_5 + 2X_6 + X_7 + X_8 + X_9 + X_{10} + 3X_{15} + 4X_{16} + 2X_{17} + 2X_{18}$
[63]	$2X_{11} + 2X_{12} + 2X_{13} + 2X_{14} + 3X_{19} + 3X_{20}$
[64]	$2X_7 + X_8 + X_9 + 2X_{10} + X_{15} + X_{16} + 3X_{17} + 3X_{18}$
[65]	$X_{11} + X_{12} + X_{13} + X_{14} + 2X_{19} + 2X_{20}$
[66]	$X_1 + X_2 + X_3 + X_4 + X_5 + X_6 + X_{15} + 2X_{16}$
[7]	$3X_{11} + X_{12} + 2X_{13} + 3X_{19} + 2X_{20}$
[7*]	$2X_{12} + X_{13} + 3X_{14} + 2X_{19} + 3X_{20}$
[71]	$X_2 + X_3 + X_5 + X_6 + 2X_7 + 2X_8 + 2X_9 + 2X_{10} + 4X_{15} + 4X_{16} + 4X_{17} + 4X_{18}$
[72]	$2X_{11} + 3X_{12} + 3X_{13} + 2X_{14} + 5X_{19} + 5X_{20}$
[73]	$X_1 + X_2 + X_3 + X_4 + X_5 + X_6 + X_7 + 2X_8 + 2X_9$ $+X_{10} + 4X_{15} + 4X_{16} + 3X_{17} + 3X_{18}$
[74]	$2X_{11} + 2X_{12} + 2X_{13} + 2X_{14} + 4X_{19} + 4X_{20}$
[75]	$X_7 + 2X_8 + 2X_9 + X_{10} + 2X_{15} + 2X_{16} + 3X_{17} + 3X_{18}$
[76]	$X_{11} + 2X_{12} + 2X_{13} + X_{14} + 2X_{19} + 2X_{20}$
[77]	$X_2 + X_3 + X_5 + X_6 + 2X_{15} + 2X_{16}$

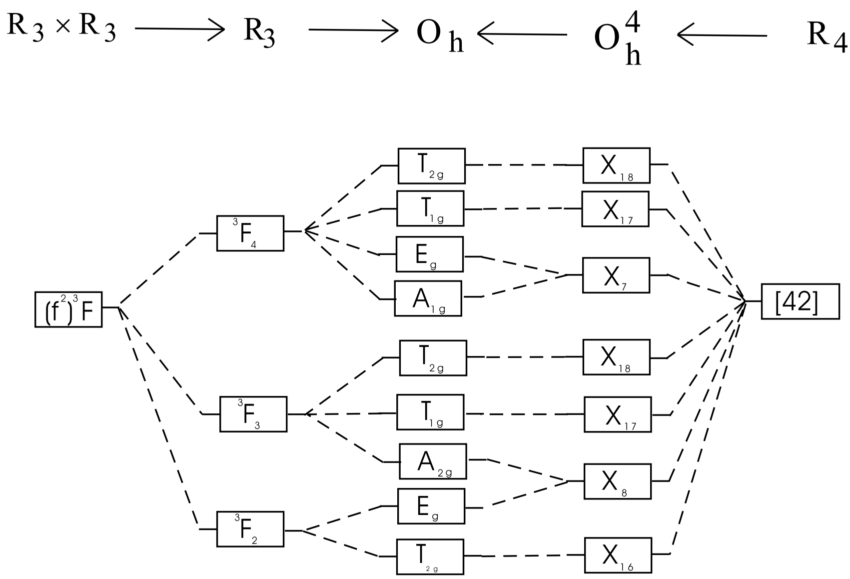

Fig. 2. Hypercubic classification of the state ^3F of f^2 configuration in cubic crystal.

for these elements:

$$\chi[j_1, j_2]^* = -\chi[j_1, j_2] \tag{11}$$

The branching relations for the reduction of IRs of group O_4 on the group O_h^4 are presented in Table VIII.

6. EXAMPLE AND DISCUSSION

The example of application of reduction relations for the term ^3F of f^2 configuration is shown in Fig. 1. If the spin and orbital parts are independent, the total symmetry group of the state with $L = 3$ and $S = 1$ is the direct product of two rotational groups $R_3 \times R_3$. When the spin-orbit interaction is taken into account the symmetry group is reduced to R_3 and one obtains three states $^3F_4$, $^3F_3$, and $^3F_2$, labelled by the total angular momentum J. In cubic crystal field these wavefunctions are split on the states belonging to IRs of O_h group. There are many repeating IRs in the final state of reduction and additional quantum numbers are required. The hypercubic classification is shown on the right part of this figure. The state with $L = 3$ and $S = 1$ belongs to the IR (Wybourne, 1973) of four-dimensional orthogonal group. The reduction of this IR on the group O_h^4 is shown in this figure. Note that when IRs X_9 and X_{10} are reduced on O_h group only odd IRs appear (see Table VI). In our case of two-electron configuration only even IRs appear and IRs X_9 and X_{10} are not shown in Fig. 2. It is seen from this figure IRs T_{2g} originate from IRs X_{16} or X_{18} of hypercube and their labels may be used as additional quantum numbers as T_{2g} (X_{16}) and T_{2g} (X_{18}). Also repeating IRs E_g originate from IRs X_7 and X_8 of hypercube and two repeating IRs may be labelled as $E_g(X_7)$ and $E_g(X_8)$.

7. CONCLUSION

The characters of single-valued representations of hypercubic subgroups O^4, T_d^4, T_h^4 and T^4 are obtained. Making use of representation of hypercubic group elements as rotations around two axes we obtained the reduction relations for the representation of the four-dimensional rotation group on the hypercubic group. This relations are used to obtain a new hypercubic classification of many-electron states. It is shown that hypercubic classification of many-electron states in crystals results in additional quantum number—the index of IR of hypercubic group.

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