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Irreducible Bases and Correlations of Spin States for Double Point Groups

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In terms of the irreducible bases of the group space of the octahedral double group $\mathbf{O}'$ an analytic formula is obtained to combine the spin states $|j, \mu\rangle$ into the symmetrical adapted bases belonging to a given row of a given irreducible representation of $\mathbf{O}'$. This method is effective for all double point groups. However, for the subgroups of $\mathbf{O}'$ there is another way to obtain those combinations. As an example, the correlations of spin states for the tetrahedral double group $\mathbf{T}'$ are calculated explicitly.

1. INTRODUCTION

It is a common problem to combine the spin states $|j, \mu\rangle$ into the symmetrical adapted bases (SAB) that are defined as the orthogonal bases belonging to the given rows of the given irreducible representations of a point group. The SAB are very useful in classifying the electronic states in the presence of spin coupling. In particular, for the electronic states with half-odd-integer spin, one has to deal with the double group symmetry (Bethe, 1929).

As is well known, the $SU(2)$ group is the covering group of the rotation group $SO(3)$, and provides double-valued representations of $SO(3)$. Following the homomorphism of $SU(2)$ onto $SO(3)$,

$$\pm u(\hat{\mathbf{n}}, \omega) \rightarrow R(\hat{\mathbf{n}}, \omega) \tag{1}$$

we are able to define the double point groups as follows. In the rotation group $SO(3)$, a rotation through 2π is equal to the identity E, but it is different from the identity in the $SU(2)$ group:

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$$R(\hat{\mathbf{n}}, 2\pi) = E, \qquad u(\hat{\mathbf{n}}, 2\pi) \equiv E' = -1 \tag{2}$$

The point group G is a subgroup of $SO(3)$, and the double point group G' is that of $SU(2)$. A point group G is extended into a double point group G' (Bethe, 1929) by introducing a new element E' satisfying

$$RE' = E'R, \qquad (E')^2 = E, \qquad R \in G \subset G', \quad E'R \in G' \tag{3}$$

In order to distinguish $R \in G \subset G'$ from $E'R \in G'$, we restrict the rotation angle ω to be not larger than π:

$$\begin{aligned} u(\hat{\mathbf{n}}, \omega) &\to R(\hat{\mathbf{n}}, \omega) \in G, \qquad 0 \le \omega \le \pi \\ -u(\hat{\mathbf{n}}, \omega) = u(-\hat{\mathbf{n}}, 2\pi - \omega) &\to R(-\hat{\mathbf{n}}, 2\pi - \omega) = R(\hat{\mathbf{n}}, \omega - 2\pi) \\ &= E'R(\hat{\mathbf{n}}, \omega) \end{aligned} \tag{4}$$

The period of ω in the $SU(2)$ group is 4π.

Recently, the problem of combining the spin states $|j, \mu\rangle$ into the SAB has drawn the attention of physicists. A new technique (Chen and Fan, 1997), called the double-induced technique, was used for calculating the irreducible bases for the tetrahedral group $\mathbf{T}'$ and the combinations of the angular momentum states. It was stated (Chen and Fan, 1997) that this technique can be used to calculate similar problems for the octahedral double group $\mathbf{O}'$ and icosahedral double group $\mathbf{I}'$. The character table and the correlation tables relevant for the icosahedral double group $\mathbf{I}'_h$ were presented (Balasubramanian, 1996). The element E' was denoted by R in Balasubramanian (1996) and Hamermesh (1962), and by θ in Chen and Fan (1997). The double point group G' was denoted by $G^\dagger$ in Chen and Fan (1997).

As is well known, the character tables of double point groups are easy to obtain from group theory, and the calculation for the correlation tables is straightforward. In principle, the character table can be used to find the similarity transformation that combines the states with a given angular momentum into the SAB. However, it becomes a tedious task when the angular momentum increases. Fortunately, the difficulty can be overcome by using irreducible bases in the group space.

From group theory (Hamermesh, 1962, p. 106), the group space is the representation space of the regular representation where the natural bases are the group elements. The number of times each irreducible representation is contained in the regular representation is equal to the dimension of the representation. Reducing the regular representation, we can obtain the irreducible bases $\psi^\Gamma_{\mu\nu}$ with the following property:

$$R\psi^\Gamma_{\mu\nu} = \sum_\rho \psi^\Gamma_{\rho\nu} D^\Gamma_{\rho\mu}(R), \qquad \psi^\Gamma_{\mu\nu} R = \sum_\rho D^\Gamma_{\nu\rho}(R)\psi^\Gamma_{\mu\rho} \tag{5}$$

Therefore, those irreducible bases are called the bases belonging to the μ row and the ν column of the irreducible representation Γ.

Assume that G is a point group, which is a subgroup of the rotation group $SO(3)$. Applying its irreducible bases $\psi^{\Gamma}_{\mu\nu}$ to the angular momentum states $|j, \rho\rangle$, we obtain the SAB $\psi^{\Gamma}_{\mu\nu}|j, \rho\rangle$, if it is not vanishing, belonging to the μ row of the representation Γ of the point group G:

$$R\psi^{\Gamma}_{\mu\nu}|j, \rho\rangle = \sum_{\lambda} D^{\Gamma}_{\lambda\mu}(R)\psi^{\Gamma}_{\lambda\nu}|j, \rho\rangle \tag{6}$$

This method is effective for both integer and half-odd-integer angular momentum states. In this paper we will calculate the irreducible bases in the group space of the octahedral double group $\mathbf{O}'$ (Section 2), and then find a simple and unified formula [see (18) in Section 3] for calculating the SAB. This method is effective for all double point groups. Most double point groups are subgroups of $\mathbf{O}'$. The SAB for a subgroup can also be obtained from the SAB of $\mathbf{O}'$ by reducing the subduced representations of $\mathbf{O}'$ for the subgroup. In Section 4 we will demonstrate this method by taking the tetrahedral double group $\mathbf{T}'$ as an example. The calculation for the icosahedral double group will be published elsewhere Dong *et al.* (1997). We give some conclusions in Section 5.

2. OCTAHEDRAL DOUBLE GROUP

A cube is shown in Fig. 1. The vertices on the upper part are labeled by A_j, $1 \le j \le 4$, and their opposite vertices by B_j. The coordinate axes point from the center O to the centers of the faces, respectively.

The group $\mathbf{O}$ contains three fourfold axes, four threefold axes, and six twofold axes. The fourfold axes are along the coordinate axes, and the

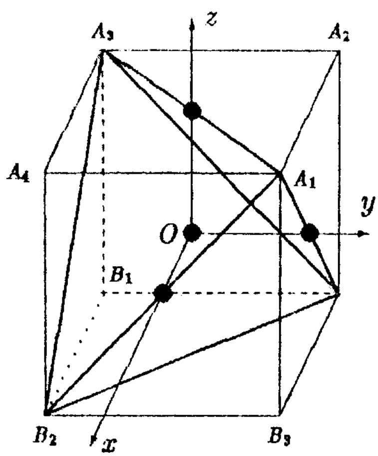

Fig. 1. A cube with $\mathbf{O}_h$ symmetry.

rotations through $\pi/2$ around those fourfold axes are denoted by T_x, T_y, and T_z, respectively. The threefold axes point from B_j to A_j ($1 \leq j \leq 4$) with the polar angle θ and azimuthal angles φ_j:

$$\cos\theta = \sqrt{1/3}, \qquad \varphi_j = (2j - 1)\pi/4, \qquad 1 \leq j \leq 4 \tag{7}$$

The rotations through $2\pi/3$ around those threefold axes are denoted by R_j, $1 \leq j \leq 4$. The twofold axes join the midpoints of two opposite edges, and corresponding rotations are denoted by S_j, $1 \leq j \leq 6$. The polar and azimuthal angles of the first four axes are $\pi/4$ and $(j - 1)\pi/2$, and the last two axes are located on the xy plane with the azimuthal angles $\pi/4$ and $3\pi/4$, respectively.

The octahedral double group $\mathbf{O}'$ contains 48 elements and eight classes. There are eight inequivalent irreducible representations for $\mathbf{O}'$: Five representations D^{A_1}, D^{A_2}, D^{E}, D^{T_1}, and D^{T_2} are called single-valued ones, and three representations $D^{E_1'}$, $D^{E_2'}$, and $D^{G'}$ are double-valued ones. From a standard calculation of group theory, the character table is obtained and listed in Table I. The row (column) index μ runs over integer (in a single-valued representation) or half-odd integer (in a double-valued one). The order of the row index μ is also listed in Table 1.

The octahedral double group $\mathbf{O}_h'$ is the direct product of $\mathbf{O}'$ and the inversion group $\{E, P\}$, where P is the inversion operator. According to the parity, the irreducible representations of $\mathbf{O}_h'$ are denoted as Γ_g (even) and Γ_u (odd), respectively. In this paper we will pay more attention to the double group $\mathbf{O}'$.

The rank of the double group $\mathbf{O}'$ is three. We choose E', T_z, and S_1 as the generators of $\mathbf{O}'$. The representation matrix of E' is equal to the unit matrix 1 in a single-valued irreducible representation and -1 in a double-valued one. It is convenient to choose the bases in an irreducible representations of $\mathbf{O}'$ such that the representation matrices of the generator T_z are diagonal with the diagonal elements η^{μ}, where $\eta = \exp\{-i\pi/2\}$. Assume

Table I. Character Table of the Octahedral Double Group $\mathbf{O}'$

	E	$6C_4$	$6C_4^2$	$8C_3$	$12C_2$	E'	$6C_4^3$	$8C_3^2$	μ
A_1	1	1	1	1	1	1	1	1	0
A_2	1	-1	1	1	-1	1	-1	1	2
E	2	0	2	-1	0	2	0	-1	2, 0
T_1	3	1	-1	0	-1	3	1	0	1, 0, -1
T_2	3	-1	-1	0	1	3	-1	0	3, 2, 1
E_1'	2	$\sqrt{2}$	0	1	0	-2	$-\sqrt{2}$	-1	1/2, $-1/2$
E_2'	2	$-\sqrt{2}$	0	1	0	-2	$\sqrt{2}$	-1	3/2, $-3/2$
G'	4	0	0	-1	0	-4	0	1	3/2, 1/2, $-1/2$, $-3/2$

that the bases $\Phi_{\mu\nu}$ in the $\mathbf{O}'$ group space are the eigenstates of left-action and right-action of T_z:

$$T_z\Phi_{\mu\nu} = \eta^{\mu}\Phi_{\mu\nu}, \qquad \Phi_{\mu\nu}T_z = \eta^{\nu}\Phi_{\mu\nu} \tag{8}$$

The bases $\Phi_{\mu\nu}$ can be easily calculated by the projection operator P_μ (Hamermesh, 1962, p. 113):

$$\Phi_{\mu\nu} = cP_\mu RP_\nu, \qquad P_\mu = \frac{E + \eta^{-4\mu}E'}{8}\sum_{a=0}^{3}\eta^{-\mu a}T_z^a \tag{9}$$

where c is a normalization factor. The choice of the group element R in (9) will not affect the results except for the factor c. The subscripts μ and ν should be integer or half-odd integer, simultaneously. In the following we choose E, T_x^2, and S_1 as the group element R in (9), respectively, and obtain three independent sets of bases $\Phi_{\mu\nu}^{(i)}$:

$$\begin{aligned}
\Phi_{\mu\mu}^{(1)} &= \frac{E + \eta^{-4\mu}E'}{2\sqrt{2}}\sum_{a=0}^{3}\eta^{-\mu a}T_z^a \\
\Phi_{\mu\bar{\mu}}^{(2)} &= \frac{E + \eta^{-4\mu}E'}{2\sqrt{2}}\sum_{a=0}^{3}\eta^{-\mu a}T_z^aT_x^2 \\
&= \frac{E + \eta^{-4\mu}E'}{2\sqrt{2}}(T_x^2 + \eta^{-\mu}S_5 + \eta^{-2\mu}T_y^2 + \eta^{-3\mu}S_6) \\
\Phi_{\mu\nu}^{(3)} &= \frac{E + \eta^{-4\mu}E'}{4\sqrt{2}}\sum_{a=0}^{3}\eta^{-\mu a}T_z^aS_1\sum_{b=0}^{3}\eta^{-\nu b}T_z^b \\
&= \frac{E + \eta^{-4\mu}E'}{4\sqrt{2}}\{(S_1 + \eta^{-\mu}R_1^2 + \eta^{-2\mu}T_y^3 + \eta^{\mu}R_4) \\
&\quad + \eta^{(\mu-\nu)}(S_4 + \eta^{-\mu}R_4^2 + \eta^{-2\mu}T_x^3 + \eta^{\mu}R_3) \\
&\quad + \eta^{2(\mu-\nu)}(S_3 + \eta^{-\mu}R_3^2 + \eta^{2\mu}T_y + \eta^{\mu}R_2) \\
&\quad + \eta^{3(\mu-\nu)}(S_2 + \eta^{-\mu}R_2^2 + \eta^{2\mu}T_x + \eta^{\mu}R_1)\}
\end{aligned} \tag{10}$$

where and hereafter the subscript $\bar{\mu}$ denotes $-\mu$. Those bases $\Phi_{\mu\nu}^{(i)}$ should be combined into the irreducible bases $\psi_{\mu\nu}^{\Gamma}$ belonging to the given irreducible representation Γ. The combinations can be determined from the condition that the irreducible bases should be the eigenstate of a class operator W, which was called CSCO-I in Chen and Fan (1997). The eigenvalues α_Γ can be calculated [see (3-170) in Hamermesh (1962)] from the characters in the irreducible representations Γ listed in Table I:

$$W = T_x + T_y + T_z + E'T_x^3 + E'T_y^3 + E'T_z^3, \qquad W\psi^\Gamma_{\mu\nu} = \psi^\Gamma_{\mu\nu}W = \alpha_\Gamma\psi^\Gamma_{\mu\nu}$$

$$\begin{array}{llll} \alpha_{A_1} = 6, & \alpha_{A_2} = -6, & \alpha_E = 0, & \alpha_{T_1} = 2, \\ \alpha_{T_2} = -2, & \alpha_{E_1'} = 3\sqrt{2}, & \alpha_{E_2'} = -3\sqrt{2}, & \alpha_{G'} = 0 \end{array} \tag{11}$$

Although a coincidence occurs, $\alpha_E = \alpha_{G'}$, this coincidence will not constitute an obstacle to calculation, because D^E is a single-valued representation, but $D^{G'}$ is a double-valued one.

Now we are able to calculate the matrix form of W in the bases $\Phi^{(i)}_{\mu\nu}$, and diagonalize it. The $\psi^\Gamma_{\mu\nu}$ are just the eigenvectors of the matrix form of W:

$$\psi^\Gamma_{\mu\nu} = N^{-1/2} \sum_{i=1}^{3} C_i \Phi^{(i)}_{\mu\nu} \tag{12}$$

where N is the normalization factor.

In these irreducible bases the representation matrices of E' and T_z are diagonal with the diagonal elements ± 1 and η^μ, respectively. But the explicit matrix forms of another generator S_1 will depend upon the phases of the bases $\psi^\Gamma_{\mu\nu}$. We choose the phases such that S_1 has the following representation matrices:

$$\begin{gathered} D^{A_1}(S_1) = -D^{A_2}(S_1) = 1, \qquad D^E(S_1) = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \\ D^{T_1}(S_1) = -D^{T_2}(S_1) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{2} & -1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ -1 & \sqrt{2} & -1 \end{pmatrix} \\ D^{E_1'}(S_1) = \frac{i}{\sqrt{2}}\begin{pmatrix} -1 & -1 \\ -1 & 1 \end{pmatrix}, \qquad D^{E_2'}(S_1) = \frac{i}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \\ D^{G'}(S_1) = \frac{i}{2\sqrt{2}}\begin{pmatrix} 1 & \sqrt{3} & \sqrt{3} & 1 \\ \sqrt{3} & 1 & -1 & -\sqrt{3} \\ \sqrt{3} & -1 & -1 & \sqrt{3} \\ 1 & -\sqrt{3} & \sqrt{3} & -1 \end{pmatrix} \end{gathered} \tag{13}$$

Some representations coincide with the subduced representations of D^j of $SO(3)$:

$$\begin{array}{ll} D^{A_1}(R) = D^0(R), & D^{T_1}(R) = D^1(R) \\ D^{E_1'}(R) = D^{1/2}(R), & D^{G'}(R) = D^{3/2}(R) \end{array} \qquad R \in \mathbf{O}' \tag{14}$$

The normalization factors N and combination coefficients C_i in the irreducible bases (12) are listed in Table II.

Table II. Irreducible Bases in the Group Space of **O′**

$$\psi^{\Gamma}_{\mu\nu} = N^{-1/2}\{C_1\Phi^{(1)}_{\mu\nu} + C_2\Phi^{(2)}_{\mu\nu} + C_3\Phi^{(3)}_{\mu\nu}\}$$

$$\psi^{A1}_{00} = \{\Phi^{(1)}_{00} + \Phi^{(2)}_{00} + 2\Phi^{(3)}_{00}\}/\sqrt{6}$$

$$\psi^{A2}_{22} = \{\Phi^{(1)}_{22} + \Phi^{(2)}_{22} - 2\Phi^{(3)}_{22}\}/\sqrt{6}$$

Γ = *E*						Γ = *E*					
μ	ν	C_1	C_2	C_3	N	μ	ν	C_1	C_2	C_3	N
2	2	1	1	1	3	2	0			1	1
0	2			1	1	0	0	1	1	−1	3

Γ = T_1						Γ = T_2					
μ	ν	C_1	C_2	C_3	N	μ	ν	C_1	C_2	C_3	N
1	1	1		−1	2	3	3	1		1	2
0	1			−1	1	2	3			1	1
$\bar{1}$	1		−1	−1	2	1	3		−1	1	2
1	0			−1	1	3	2			1	1
0	0	1	−1		2	2	2	1	−1		2
$\bar{1}$	0			1	1	1	2			−1	1
1	$\bar{1}$		−1	−1	2	3	1		−1	1	2
0	$\bar{1}$			1	1	2	1			−1	1
$\bar{1}$	$\bar{1}$	1		−1	2	1	1	1		1	2

Γ = E'_1						Γ = E'_2					
2μ	2ν	C_1	C_2	C_3	N	2μ	2ν	C_1	C_2	C_3	N
1	1	i		$-\sqrt{2}$	3	3	3	i		$-\sqrt{2}$	3
$\bar{1}$	1		−1	$-\sqrt{2}$	3	$\bar{3}$	3		−1	$\sqrt{2}$	3
1	$\bar{1}$		−1	$-\sqrt{2}$	3	3	$\bar{3}$		−1	$\sqrt{2}$	3
$\bar{1}$	$\bar{1}$	i		$\sqrt{2}$	3	$\bar{3}$	$\bar{3}$	i		$\sqrt{2}$	3

Γ = G'						Γ = G'					
2μ	2ν	C_1	C_2	C_3	N	2μ	2ν	C_1	C_2	C_3	N
3	3	$i\sqrt{2}$		1	3	3	$\bar{1}$			1	1
1	3			1	1	1	$\bar{1}$		$\sqrt{2}$	−1	3
$\bar{1}$	3			1	1	$\bar{1}$	$\bar{1}$	$i\sqrt{2}$		−1	3
$\bar{3}$	3		$\sqrt{2}$	1	3	$\bar{3}$	$\bar{1}$			1	1
3	1			1	1	3	$\bar{3}$		$\sqrt{2}$	1	3
1	1	$i\sqrt{2}$		1	3	1	$\bar{3}$			−1	1
$\bar{1}$	1		$\sqrt{2}$	−1	3	$\bar{1}$	$\bar{3}$			1	1
$\bar{3}$	1			1	1	$\bar{3}$	$\bar{3}$	$i\sqrt{2}$		−1	3

Now, the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ satisfy (5). The irreducible bases of the group $\mathbf{O}'_h$ can be expressed as follows:

$$\psi^{\Gamma_g}_{\mu\nu} = 2^{-1/2}(E + P)\psi^{\Gamma}_{\mu\nu}, \qquad \psi^{\Gamma_u}_{\mu\nu} = 2^{-1/2}(E - P)\psi^{\Gamma}_{\mu\nu} \tag{15}$$

3. APPLICATIONS TO THE ANGULAR MOMENTUM STATES

Due to the properties (5), we can obtain the SAB by applying $\psi^{\Gamma}_{\mu\nu}$ to any function. As an important application, we apply $\psi^{\Gamma}_{\mu\nu}$ to the angular momentum states $|j, \mu\rangle$, where the Condon–Shortley definition is used:

$$R|j, \mu\rangle = \sum_{\nu=-j}^{j} D^{j}_{\nu\mu}(R)|j, \nu\rangle, \qquad R \in SO(3) \quad \text{or} \quad SU(2) \tag{16}$$

When j is an integer l, $|l, m\rangle$ is just the spherical harmonics $Y^{l}_{m}(\theta, \varphi)$.

From (16) and the definitions of the group elements we have

$$\begin{aligned} E'|j, \mu\rangle &= (-1)^{2j}|j, \mu\rangle, \qquad T_z|j, \mu\rangle = \eta^{\mu}|j, \mu\rangle \\ T^2_x|j, \mu\rangle &= \sum_{\nu} D^{j}_{\nu\mu}(0, \pi, \pi)|j, \nu\rangle = (-1)^{j-\mu}\eta^{2\mu}|j, -\mu\rangle \\ S_1|j, \mu\rangle &= \sum_{\nu} D^{j}_{\nu\mu}(0, \pi/2, \pi)|j, \nu\rangle = \sum_{\nu} \eta^{2\mu} d^{j}_{\nu\mu}(\pi/2)|j, \nu\rangle \end{aligned} \tag{17}$$

Now, it is easy to obtain the combinations of the angular momentum states $\psi^{\Gamma}_{\mu\lambda}|j, \rho\rangle$ to the SAB of $\mathbf{O}'$:

$$\begin{aligned} \psi^{\Gamma}_{\mu\lambda}|j, \rho\rangle = \sqrt{8/N}\delta'_{\lambda\rho} \sum_{\rho} \delta'_{\mu\nu}|j, \nu\rangle\{C_1\delta_{\rho\nu} + C_2\delta_{\bar{\rho}\nu}(-1)^{j-\rho}\eta^{2\rho} \\ + 2C_3\eta^{2\rho}d^{j}_{\nu\rho}(\pi/2)\} \end{aligned} \tag{18}$$

where N and C_i were given in Table II, $\eta = \exp\{-i\pi/2\}$, and $\delta'_{\lambda\rho}$ is defined as follows:

$$\delta'_{\lambda\rho} = \begin{cases} 1 & \text{when} \quad (\lambda - \rho)/n = \text{integer} \\ 0 & \text{otherwise} \end{cases} \tag{19}$$

where $n = 4$ for $\mathbf{O}'$, due to $\eta^4 = 1$. In driving (18) some terms were merged, so that the functions need to be normalized again.

Equation (18) is a simple and unified formula for calculating the correlations of the spin states. For fixed λ and ρ satisfying $\delta'_{\lambda\rho} = 1$, we obtain the combinations of the angular momentum states $\psi^{\Gamma}_{\mu\lambda}|j, \rho\rangle$ belonging to the μ

row of the irreducible representation Γ of $\mathbf{O}'$. Different choice of λ and ρ may cause the combinations to vanish, to be dependent on each other, or to be independent. The number of independent combinations depends upon the number of times the irreducible representation Γ of $\mathbf{O}'$ is contained in the subduced representation of D^j of $SU(2)$. The latter is completely determined by the characters of the representations Γ and D^j.

Those combinations given in (18) are very easy to calculate, by a simple computer file or even by hand. In the following we list some combinations as examples:

$$\psi^{A_1}_{00}\,|0,\,0\rangle = 4\sqrt{3}\,|0,\,0\rangle, \qquad \psi^{T_1}_{\mu 1}\,|1,\,1\rangle = 4\,|1,\,\mu\rangle$$

$$\psi^{E}_{22}\,|2,\,2\rangle = 2\sqrt{3}\,\left(\sqrt{1/2}\,|2,\,2\rangle + \sqrt{1/2}\,|2,\,-2\rangle\right)$$

$$\psi^{E}_{02}\,|2,\,2\rangle = 2\sqrt{3}\,|2,\,0\rangle$$

$$\psi^{T_2}_{3\bar{2}}\,|2,\,2\rangle = 2\sqrt{2}\,|2,\,-1\rangle$$

$$\psi^{T_2}_{2\bar{2}}\,|2,\,2\rangle = 2\sqrt{2}\,\left(\sqrt{1/2}\,|2,\,2\rangle - \sqrt{1/2}\,|2,\,-2\rangle\right)$$

$$\psi^{T_2}_{1\bar{2}}\,|2,\,2\rangle = 2\sqrt{2}\,\left(-|2,\,1\rangle\right)$$

$$\psi^{A_2}_{2\bar{2}}\,|3,\,2\rangle = 2\sqrt{6}\,\left(\sqrt{1/2}\,|3,\,2\rangle - \sqrt{1/2}\,|3,\,-\,2\rangle\right)$$

$$\psi^{T_1}_{1\bar{1}}\,|3,\,3\rangle = \sqrt{10}\,\left(\sqrt{3/8}\,|3,\,1\rangle + \sqrt{5/8}\,|3,\,-3\rangle\right)$$

$$\psi^{T_1}_{0\bar{1}}\,|3,\,3\rangle = \sqrt{10}\,\left(-|3,\,0\rangle\right)$$

$$\psi^{T_1}_{\bar{1}\bar{1}}\,|3,\,3\rangle = \sqrt{10}\,\left(\sqrt{5/8}\,|3,\,3\rangle + \sqrt{3/8}\,|3,\,-1\rangle\right)$$

$$\psi^{T_2}_{3\bar{3}}\,|3,\,3\rangle = -\sqrt{6}\,\left(-\sqrt{3/8}\,|3,\,3\rangle + \sqrt{5/8}\,|3,\,-1\rangle\right)$$

$$\psi^{T_2}_{2\bar{3}}\,|3,\,3\rangle = -\sqrt{6}\,\left(\sqrt{1/2}\,|3,\,2\rangle + \sqrt{1/2}\,|3,\,-2\rangle\right)$$

$$\psi^{T_2}_{1\bar{3}}\,|3,\,3\rangle = -\sqrt{6}\,\left(\sqrt{5/8}\,|3,\,1\rangle - \sqrt{3/8}\,|3,\,-3\rangle\right)$$

$$\psi^{E_1'}_{\mu(1/2)}\,|1/2,\,1/2\rangle = i2\sqrt{6}\,|1/2,\,\mu\rangle$$

$$\psi^{G'}_{\mu(3/2)}\,|3/2,\,3/2\rangle = i2\sqrt{3}\,|3/2,\,\mu\rangle$$

$$\psi^{E_2'}_{(3/2)\overline{(3/2)}}\,|5/2,\,5/2\rangle = i2\left(-\sqrt{5/6}\,|5/2,\,3/2\rangle + \sqrt{1/6}\,|5/2,\,-5/2\rangle\right)$$

$$\psi^{E_2'}_{\overline{(3/2)}\,\overline{(3/2)}}\,|5/2,\,5/2\rangle = i2\left(\sqrt{1/6}\,|5/2,\,5/2\rangle - \sqrt{5/6}\,|5/2,\,-3/2\rangle\right)$$

$$\psi^{G'}_{(3/2)\overline{(3/2)}}\,|5/2,\,5/2\rangle = i\sqrt{10}\,\left(-\sqrt{1/6}\,|5/2,\,3/2\rangle - \sqrt{5/6}\,|5/2,\,-5/2\rangle\right)$$

$$\psi^{G'}_{(1/2)\overline{(3/2)}}\,|5/2,\,5/2\rangle = i\sqrt{10}\,|5/2,\,1/2\rangle,$$

$$\psi^{G'}_{\overline{(1/2)}\,\overline{(3/2)}}\,|5/2,\,5/2\rangle = i\sqrt{10}\,\left(-|5/2,\,-1/2\rangle\right)$$

$$\psi^{G'}_{(3/2)\overline{(3/2)}}|5/2,\ 5/2\rangle = i\sqrt{10}\ (\sqrt{5/6}\ |5/2,\ 5/2\rangle + \sqrt{1/6}\ |5/2,\ -3/2\rangle)$$

4. TETRAHEDRAL DOUBLE GROUP

The tetrahedral double group $\mathbf{T}'$ is a subgroup of $\mathbf{O}'$ with the generators E', T_z^2, and R_1:

$$R_1 = E'S_1T_z^3 = S_1T_z^{-1} \tag{20}$$

In the irreducible bases we choose, the representation matrices of E' and T_z^2 are diagonal with the diagonal elements ± 1 and $\eta^{2\mu}$, respectively, and the representation matrices of R_1 are as follows:

$$D^{A_0}(R_1) = 1, \qquad D^{A_+}(R_1) = \omega = \exp\{-i2\pi/3\},$$

$$D^{A_-}(R_1) = \overline{\omega} = \exp\{i2\pi/3\}$$

$$D^T(R_1) = \frac{1}{2}\begin{pmatrix} -i & -\sqrt{2} & i \\ -i\sqrt{2} & 0 & -i\sqrt{2} \\ -i & \sqrt{2} & i \end{pmatrix}, \qquad D^{E_0'}(R_1) = \frac{\tau}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \tag{21}$$

$$D^{E_+'}(R_1) = \omega D^{E_0'}(R_1), \qquad D^{E_-'}(R_1) = \overline{\omega} D^{E_0'}(R_1)$$

where $\tau = \exp\{-i\pi/4\}$. The character table of $\mathbf{T}'$ is given in Table III.

Generally speaking, an irreducible representation of $\mathbf{O}'$ is a reducible one as a subduced representation of $\mathbf{T}'$. Through the following similarity transformation, the SAB of $\mathbf{O}'$ can be further combined into the SAB of $\mathbf{T}'$:

$$D^{A_1}(R), \qquad D^{A_2}(R) \to D^{A_0}(R)$$

$$X_1^{-1}D^E(R)X_1 \to D^{A_+}(R) \oplus D^{A_-}(R)$$

$$D^{T_1}(R), \qquad D^{T_2}(R) \to D^T(R)$$

Table III. Character Table of the Tetrahedral Double Group $\mathbf{T}'$
$\omega = (\omega)^{-1} = \exp\{-i2\pi/3\}$

	E	$4C_3$	$4C_3^2$	$6C_2$	E'	$4C_3^4$	$4C_3^5$	μ
A_0	1	1	1	1	1	1	1	0
A_+	1	ω	ω	1	1	ω	ω	0
A_-	1	ω	ω	1	1	ω	ω	0
T	3	0	0	-1	3	0	0	$1, 0, -1$
E_0'	2	1	-1	0	-2	-1	1	$1/2, -1/2$
E_+'	2	ω	$-\omega$	0	-2	$-\omega$	ω	$1/2, -1/2$
E_-'	2	ω	$-\omega$	0	-2	$-\omega$	ω	$1/2, -1/2$

$$D^{E_1'}(R),\ X_2^{-1}D^{E_2'}(R)X_2 \to D^{E_0'}(R)$$

$$X_3^{-1}D^{G'}(R)X_3 \to D^{E_+'}(R) \oplus D^{E_-'}(R)$$

$$X_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}, \qquad X_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{22}$$

$$X_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 & 1 \\ i & 0 & -i & 0 \\ 0 & -i & 0 & i \\ -1 & 0 & -1 & 0 \end{pmatrix}$$

For example,

$$\begin{aligned}
\psi_{00}'^{A+}|2, 2\rangle &= \{\psi_{22}^{E}|2, 2\rangle - i\psi_{02}^{E}|2, 2\rangle\}/\sqrt{2} \\
&\sim \{|2, 2\rangle - i\sqrt{2}|2, 0\rangle + |2, -2\rangle\}/2 \\
\psi_{00}'^{A-}|2, 2\rangle &= \{\psi_{22}^{E}|2, 2\rangle + i\psi_{02}^{E}|2, 2\rangle\}/\sqrt{2} \\
&\sim \{|2, 2\rangle + i\sqrt{2}|2, 0\rangle + |2, -2\rangle\}/2 \qquad (23)\\
\psi_{10}'^{T}|2, 2\rangle &= \psi_{32}^{T_2}|2, 2\rangle \sim |2, -1\rangle \\
\psi_{00}'^{T}|2, 2\rangle &= \psi_{22}^{T_2}|2, 2\rangle \sim \{|2, 2\rangle - |2, -2\rangle\}/\sqrt{2} \\
\psi_{10}'^{T}|2, 2\rangle &= \psi_{12}^{T_2}|2, 2\rangle \sim -|2, 1\rangle
\end{aligned}$$

As an alternative method, (23) can also be obtained from the irreducible bases of the group space of $\mathbf{T}'$. Similar to (9) and (10), we calculate the bases $\Phi_{\mu\nu}'^{(i)}$ by the projection operator P_μ':

$$\Phi_{\mu\nu}' = cP_\mu' RP_\nu', \qquad P_\mu' = \frac{1}{4}(E + \eta^{-4\mu}E')(E + \eta^{-2\mu}T_z^2) \tag{24}$$

We choose E, T_x^2, R_1, and R_1^2 as the group element R in (24), respectively, and obtain four independent sets of bases $\Phi_{\mu\nu}'^{(i)}$:

$$\begin{aligned}
\Phi_{\mu\mu}'^{(1)} &= \frac{E + \eta^{4\mu}E'}{2}(E + \eta^{-2\mu}T_z^2) \\
\Phi_{\mu\mu}'^{(2)} &= \frac{E + \eta^{4\mu}E'}{2}(T_x^2 + \eta^{-2\mu}T_y^2) \qquad (25)\\
\Phi_{\mu\nu}'^{(3)} &= \frac{E + \eta^{4\mu}E'}{2\sqrt{2}}(R_1 + \eta^{-2\mu}R_2^2 + \eta^{2(\mu-\nu)}R_3 + \eta^{-2\nu}R_4^2)
\end{aligned}$$

$$\Phi'^{(4)}_{\mu\nu} = \frac{E + \eta^{4\mu}E'}{2\sqrt{2}} (R_1^2 + \eta^{2\mu}R_4 + \eta^{2(\mu-\nu)}R_3^2 + \eta^{2\nu}R_2)$$

The class operator W' is used to determine the irreducible bases $\psi'^{\Gamma}_{\mu\nu}$:

$$\begin{gathered} W' = R_1 + R_3 + E'R_1^2 + E'R_3^2, \qquad W'\psi'^{\Gamma}_{\mu\nu} = \psi'^{\Gamma}_{\mu\nu}W' = \beta_\Gamma\psi'^{\Gamma}_{\mu\nu} \\ \beta_{A_0} = 4, \qquad \beta_{A+} = 4\omega, \qquad \beta_{A-} = 4\overline{\omega}, \qquad \beta_T = 0 \\ \beta_{E'_0} = 2, \qquad \beta_{E'_+} = 2\omega, \qquad \beta_{E'_-} = 2\overline{\omega} \end{gathered} \tag{26}$$

$\psi'^{\Gamma}_{\mu\nu}$ are the eigenvectors of the matrix form of W' in the bases $\Phi'^{(i)}_{\mu\nu}$:

$$\psi'^{\Gamma}_{\mu\nu} = N^{-1/2} \sum_{i=1}^{4} C_i \Phi'^{\Gamma}_{\mu\nu} \tag{27}$$

where the normalization factor N and the combination coefficients C_i are listed in Table IV.

Recall the Eulerian angles of the relevant rotations:

$$T_x^2 = R(0, \pi, \pi), \qquad R_1 = R(0, \pi/2, \pi/2), \qquad R_1^2 = R(\pi/2, \pi/2, \pi) \tag{28}$$

Now, applying the irreducible bases $\psi'^{\Gamma}_{\mu\nu}$ to the angular momentum states $|j, \mu\rangle$, we obtain the SAB for $\mathbf{T}'$:

$$\begin{aligned} \psi'^{\Gamma}_{\mu\lambda}|j, \rho\rangle = \sqrt{4/N}\delta'_{\lambda\rho} \sum_{\nu} \delta'_{\mu\nu}|j, \nu\rangle\{C_1\delta_{\rho\nu} + C_2\delta_{\bar{\rho}\nu}(-1)^{j-\rho}\eta^{2\rho} \\ + \sqrt{2}C_3\eta^{\rho}d^j_{\nu\rho}(\pi/2) + \sqrt{2}C_4\eta^{\nu+2\rho}d^j_{\nu\rho}(\pi/2)\} \end{aligned} \tag{29}$$

where $\delta'_{\lambda\rho}$ is defined in (19) with $n = 2$.

It is very easy to calculate from (29) the combinations of the angular momentum states $|j, \mu\rangle$ to the SAB of $\mathbf{T}'$. In the following we list some examples:

$$\psi'^{A_0}_{00}|0, 0\rangle = 2\sqrt{6}\,|0, 0\rangle, \qquad \psi'^{T}_{\mu 1}|1, 1\rangle = 2\sqrt{2}\,|1, \mu\rangle$$

$$\psi'^{A+}_{00}|2, 2\rangle = \sqrt{6}((1/2)|2, 2\rangle - i\sqrt{1/2}\,|2, 0\rangle + (1/2)|2, -2\rangle)$$

$$\psi'^{A-}_{00}|2, 2\rangle = \sqrt{6}((1/2)|2, 2\rangle + i\sqrt{1/2}\,|2, 0\rangle + (1/2)|2, -2\rangle),$$

$$\psi'^{T}_{10}|2, 2\rangle = 2|2, -1\rangle,$$

$$\psi'^{T}_{00}|2, 2\rangle = 2(\sqrt{1/2}\,|2, 2\rangle - \sqrt{1/2}\,|2, -2\rangle)$$

$$\psi'^{T}_{\bar{1}0}|2, 2\rangle = 2(-|2, 1\rangle)$$

$$\psi'^{A_0}_{00}|3, 2\rangle = 2\sqrt{3}(\sqrt{1/2}\,|3, 2\rangle - \sqrt{1/2}\,|3, -2\rangle)$$

Table IV. Irreducible Bases in the Group Space of $\mathbf{T}'$

$$\psi'^{\Gamma}_{\mu\nu} = N^{-1/2} \sum_{i=1}^{4} C_i \Phi'^{(i)}_{\mu\nu}$$

$$\tau = \exp\{-i\pi/4\}, \qquad \omega = (\bar{\omega})^{-1} = \exp\{-i2\pi/3\}$$

$$\psi'^{A0}_{00} = \{\Phi^{(1)}_{00} + \Phi^{(2)}_{00} + \sqrt{2}\Phi^{(3)}_{00} + \sqrt{2}\Phi^{(4)}_{00}\}/\sqrt{6}$$

$$\psi'^{A+}_{00} = \{\Phi^{(1)}_{00} + \Phi^{(2)}_{00} + \sqrt{2}\bar{\omega}\Phi^{(3)}_{00} + \sqrt{2}\omega\Phi^{(4)}_{00}\}/\sqrt{6}$$

$$\psi'^{A-}_{00} = \{\Phi^{(1)}_{00} + \Phi^{(2)}_{00} + \sqrt{2}\omega\Phi^{(3)}_{00} + \sqrt{2}\bar{\omega}\Phi^{(4)}_{00}\}/\sqrt{6}$$

$\Gamma = T$							$\Gamma = T$						
μ	ν	C_1	C_2	C_3	C_4	N	μ	ν	C_1	C_2	C_3	C_4	N
1	1	$\sqrt{2}$		i	$-i$	4	$\bar{1}$	0			1	$-i$	2
0	1			i	-1	2	1	$\bar{1}$		$-\sqrt{2}$	$-i$	$-i$	4
$\bar{1}$	1		$-\sqrt{2}$	i	i	4	0	$\bar{1}$			i	1	2
1	0			-1	$-i$	2	$\bar{1}$	$\bar{1}$	$\sqrt{2}$		$-i$	i	4
0	0	1	-1			2							

$\Gamma = E'_0$							$\Gamma = E'_0$						
2μ	2ν	C_1	C_2	C_3	C_4	N	2μ	2ν	C_1	C_2	C_3	C_4	N
1	1	τ		1	i	3	1	$\bar{1}$		τ	1	1	3
$\bar{1}$	1		$i\tau$	1	1	3	$\bar{1}$	$\bar{1}$	$-i\tau$		1	i	3

$\Gamma = E'_+$							$\Gamma = E'_-$						
2μ	2ν	C_1	C_2	C_3	C_4	N	2μ	2ν	C_1	C_2	C_3	C_4	N
1	1	τ		$\bar{\omega}$	$i\omega$	3	1	1	τ		ω	$i\bar{\omega}$	3
$\bar{1}$	1		$i\tau$	$\bar{\omega}$	ω	3	$\bar{1}$	1		$i\tau$	ω	$\bar{\omega}$	3
1	$\bar{1}$		$i\tau$	$i\bar{\omega}$	$i\omega$	3	1	$\bar{1}$		$i\tau$	$i\omega$	$i\bar{\omega}$	3
$\bar{1}$	$\bar{1}$	τ		$-i\bar{\omega}$	$-\omega$	3	$\bar{1}$	$\bar{1}$	τ		$-i\omega$	$-\bar{\omega}$	3

$$\psi'^{T}_{11} |3, 3\rangle = -\sqrt{3}(-\sqrt{3/8}\,|3, 3\rangle + \sqrt{5/8}\,|3, -1\rangle)$$

$$\psi'^{T}_{01} |3, 3\rangle = -\sqrt{3}(\sqrt{1/2}\,|3, 2\rangle + \sqrt{1/2}\,|3, -2\rangle)$$

$$\psi'^{T}_{11} |3, 3\rangle = -\sqrt{3}(\sqrt{5/8}\,|3, 1\rangle - \sqrt{3/8}\,|3, -3\rangle)$$

$$\psi'^{T}_{11} |3, 3\rangle = \sqrt{5}(\sqrt{3/8}\,|3, 1\rangle + \sqrt{5/8}\,|3, -3\rangle)$$

$$\psi'^{T}_{01} |3, 3\rangle = \sqrt{5}(-|3, 0\rangle)$$

$$\psi'^{T}_{11} |3, 3\rangle = \sqrt{5}(\sqrt{5/8}\,|3, 3\rangle + \sqrt{3/8}\,|3, -1\rangle)$$

$$\psi'^{E'_0}_{\mu(1/2)} |1/2, 1/2\rangle = 2\sqrt{3}\tau\,|1/2, \mu\rangle$$

$$\psi'^{E'_+}_{(1/2)(\overline{1/2})}|3/2,\ 3/2\rangle = \sqrt{6}\tau(i\sqrt{1/2}\,|3/2,\ 1/2\rangle - \sqrt{1/2}\,|3/2,\ -3/2\rangle)$$

$$\psi'^{\overline{E'_+}}_{(1/2)(\overline{1/2})}|3/2,\ 3/2\rangle = \sqrt{6}\tau(\sqrt{1/2}\,|3/2,\ 3/2\rangle - i\sqrt{1/2}\,|3/2,\ -1/2\rangle)$$

$$\psi'^{E'_-}_{(1/2)(\overline{1/2})}|3/2,\ 3/2\rangle = \sqrt{6}\tau(-i\sqrt{1/2}\,|3/2,\ 1/2\rangle - \sqrt{1/2}\,|3/2,\ -3/2\rangle)$$

$$\psi'^{\overline{E'_-}}_{(1/2)(\overline{1/2})}|3/2,\ 3/2\rangle = \sqrt{6}\tau(\sqrt{1/2}\,|3/2,\ 3/2\rangle + i\sqrt{1/2}\,|3/2,\ -1/2\rangle)$$

$$\psi'^{E'_0}_{(1/2)(1/2)}|5/2,\ 5/2\rangle = \sqrt{2}\tau(\sqrt{1/6}\,|5/2,\ 5/2\rangle - \sqrt{5/6}\,|5/2,\ -3/2\rangle)$$

$$\psi'^{\overline{E'_0}}_{(1/2)(1/2)}|5/2,\ 5/2\rangle = \sqrt{2}\tau(-\sqrt{5/6}\,|5/2,\ 3/2\rangle + \sqrt{1/6}\,|5/2,\ -5/2\rangle)$$

$$\psi'^{E'_+}_{(1/2)(1/2)}|5/2,\ 5/2\rangle = \sqrt{5}\tau(\sqrt{5/12}\,|5/2,\ 5/2\rangle - i\sqrt{1/2}\,|5/2,\ 1/2\rangle + \sqrt{1/12}\,|5/2,\ -3/2\rangle)$$

$$\psi'^{\overline{E'_+}}_{(1/2)(1/2)}|5/2,\ 5/2\rangle = \sqrt{5}\tau(\sqrt{1/12}\,|5/2,\ 3/2\rangle - i\sqrt{1/2}\,|5/2,\ -1/2\rangle + \sqrt{5/12}\,|5/2,\ -5/2\rangle)$$

$$\psi'^{E'_-}_{(1/2)(1/2)}|5/2,\ 5/2\rangle = \sqrt{5}\tau(\sqrt{5/12}\,|5/2,\ 5/2\rangle + i\sqrt{1/2}\,|5/2,\ 1/2\rangle + \sqrt{1/12}\,|5/2,\ -3/2\rangle)$$

$$\psi'^{\overline{E'_-}}_{(1/2)(1/2)}|5/2,\ 5/2\rangle = \sqrt{5}\tau(\sqrt{1/12}\,|5/2,\ 3/2\rangle + i\sqrt{1/2}\,|5/2,\ -1/2\rangle \sqrt{5/12}\,|5/2,\ -5/2\rangle)$$

It is obvious that (23) coincides with these combinations.

5. CONCLUSION

The eigenstates of the Hamiltonian of a system with a given symmetry can be combined into symmetry-adapted bases (Hamermesh, 1962). From the irreducible bases in the group space of the symmetry group of the system, the symmetry-adapted bases can be calculated generally and simply. The combinations of the angular momentum states are important examples for calculating the symmetry-adapted bases. In this paper we calculate the explicit form of the irreducible bases of $\mathbf{O}'$ group space, and obtain a general formula (18) for calculating the combinations of angular momentum states into the SAB of $\mathbf{O}'$. The method is effective for all double point groups. However, most double point groups are subgroups of $\mathbf{O}'$, and the SAB of a subgroup of $\mathbf{O}'$ can also be calculated by further combining the SAB of $\mathbf{O}'$. The calculation for the icosahedral double group will be published elsewhere (Dong *et al.*, 1997).

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