Correlations of spin states
for icosahedral double group

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Abstract

The irreducible bases of the group space of the icosahedral double groups \( \Gamma' \)
and \( \Gamma'_h \) are calculated explicitly. Applying those bases on the spin states \( |j, \mu\rangle \),
we present a simple formula to combine the spin states into the symmetrical adapted
bases, belonging to a given row of a given irreducible representations of \( \Gamma' \) and \( \Gamma'_h \).

1. Introduction

Metallo-fullerenes are fullerene cages with a metal atom or atoms in the center of the
cage. Since Heath et al. \cite{1} showed that metal-containing fullerenes can be generated,
metallo-fullerenes have drawn considerable attentions of physicists and chemists. In order
to classify the electronic states of such Metallo-fullerenes in the present of spin-orbit
coupling, especially for the electronic states with half-odd-integer spin, one has to deal
with the double group symmetry \cite{2}.

Recently, the character table and the correlation tables relevant for the icosahedral
group \( \Gamma'_h \) were presented apparently \cite{3}. As is well known, the correlation tables is cal-
culated from the character table by the standard method of group theory \cite{4}. From the
correlation table the states with a low angular momentum can be combined by a similarity
transformation into a state belonging to a given row of an irreducible representation of \( \Gamma' \).
However, it becomes a tedious task while the angular momentum increases. Fortunately, the difficulty can be conquered by the irreducible bases in the group space of $\Gamma'$. In this note we present a simple formula (21) to combine the spin states into the symmetrical adapted bases, belonging to a given row of a given irreducible representations of $\Gamma$ and $\Gamma'$. The irreducible bases in the group space of $\Gamma$ and the combinations of the spin states are useful for the calculations of the vibrational and rotational problems for the carbon-60 molecule [5].

From group theory ([4] p.106), a group element $R$ plays a role of a basis in the group space, which is the representation space of the regular representation. The number of times each irreducible representation contained in the regular representation is equal to the dimension of the representation. Reducing the regular representation, we obtain the new bases $\psi^\Gamma_{\mu\nu}$ belonging to the $\mu$ ($\nu$) row of the irreducible representation $\Gamma$ in the left-(right-)action of a group element:

\[
R \psi^\Gamma_{\mu\nu} = \sum_{\rho} \psi^\Gamma_{\rho\nu} D^\Gamma_{\rho\nu}(R), \quad \psi^\Gamma_{\mu\nu} R = \sum_{\rho} D^\Gamma_{\mu\rho}(R) \psi^\Gamma_{\nu\rho}. \tag{1}
\]

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

\[
R \psi^\Gamma_{\mu\nu} |j, \rho\rangle = \sum_{\tau} D^\Lambda_{\tau\mu}(R) \psi^\Lambda_{\tau\nu} |j, \rho\rangle. \tag{2}
\]

This method is effective for both integer and half-odd-integer angular momentum states. In this note we will calculate the irreducible bases in the group space of the icosahedral double group (Sec. 2 and 3), and then, find a simple and unified formula ((21) in Sec.4) for calculating the combinations. A simple conclusion is given in Sec. 5.

Recently, we read a preprint [6] where a technique, called the double-induced technique, was used for calculating the irreducible bases for the tetrahedral group and the combinations of the angular momentum states. From the preprint we know that a similar work for the icosahedral double group is in preparation.

2. Icosahedral double group
A regular icosahedron is shown in Fig.1. The vertices on the upper part are labeled by $A_j$, $0 \leq j \leq 5$, and their opposite vertices by $B_j$. The $z$ and $y$ axes point from the center $O$ to $A_0$ and the midpoint of $A_2B_5$, respectively.

The group $I$ has 6 five-fold axes, 10 three-fold axes, and 15 two-fold axes. One of the five-fold axes directs along $z$ axis, and the rest point from $B_j$ to $A_j$ ($1 \leq j \leq 5$) with the polar angle $\theta_1$ and azimuthal angles $\varphi_j^{(1)}$. The rotations through $2\pi/5$ around those five-fold axes are denoted by $T_j$, $0 \leq j \leq 5$. The three-fold axes join the centers of two opposite faces. The polar angles of the first and last 5 axes are $\theta_2$ and $\theta_3$, respectively, and the azimuthal angles $\varphi_j^{(2)}$. The rotations through $2\pi/3$ around those three-fold axes are denoted by $R_j$, $1 \leq j \leq 10$. The two-fold axes join the midpoints of two opposite edges. The polar and azimuthal angles of the first, next and last 5 axes are $\theta_4$, $\varphi_j^{(1)}$, $\theta_5$, $\varphi_j^{(2)}$, $\pi$, and $\varphi_j^{(3)}$, respectively. The rotations through $\pi$ around those two-fold axes are denoted by $S_j$, $1 \leq j \leq 15$. Those angles $\theta_i$ and $\varphi_j^{(i)}$ are given as follows:

\begin{align*}
\tan \theta_1 &= 2, & \tan \theta_2 &= 3 - \sqrt{5}, & \tan \theta_3 &= 3 + \sqrt{5}, \\
\tan \theta_4 &= \left(\sqrt{5} - 1\right)/2, & \tan \theta_5 &= \left(\sqrt{5} + 1\right)/2, \\
\varphi_j^{(1)} &= 2(j - 1)\pi/5, & \varphi_j^{(2)} &= (2j - 1)\pi/5, & \varphi_j^{(3)} &= (4j - 3)\pi/10.
\end{align*}

As is well known, $SU(2)$ group is the covering group of the rotation group $SO(3)$, and provides the double-valued representations of $SO(3)$. In order to classify the angular momentum states with half-odd-integer spin, we have to extend the point group to the double point group, following the homomorphism of $SU(2)$ onto $SO(3)$:

$$\pm u(\hat{n}, \omega) \rightarrow R(\hat{n}, \omega).$$

In the rotation group $SO(3)$, a rotation through $2\pi$ is equal to identity $E$, but it is different from identity in the $SU(2)$ group:

$$R(\hat{n}, 2\pi) = E, \quad u(\hat{n}, 2\pi) \equiv E' = -1.$$  

Similarly, a point group $G$ is extended into a double point group $G'$ by introducing a new element $E'$, satisfying:

$$RE' = E'R, \quad (E')^2 = E, \quad R \in G \subset G', \quad E'R \in G'.$$
The point group $G$ is a subgroup of $SO(3)$, and the double point group $G'$ is that of $SU(2)$. For definiteness, we restrict the rotation angle $\omega$ not larger than $\pi$:

$$R(\hat{n}, \omega) \rightarrow u(\hat{n}, \omega),$$
$$R(\hat{n}, \omega - 2\pi) = R(-\hat{n}, 2\pi - \omega) \rightarrow u(-\hat{n}, 2\pi - \omega) = -u(\hat{n}, \omega), \quad 0 \leq \omega \leq \pi. \quad (7)$$

The period of $\omega$ in $SU(2)$ group is $4\pi$. The element $E'$ was denoted by $R$ in [3] and [4], and by $\theta$ in [6]. The double point group $G'$ was denoted by $G^\dagger$ in [6].

The icosahedral double group $I'$ contains 120 elements and nine classes. There are nine inequivant irreducible representations for $I'$: Five representations $A$, $T_1$, $T_2$, $G$ and $H$ are called single-valued ones, and four representations $E'_1$, $E'_2$, $G'$ and $I'$ are double-valued ones. The row (column) index runs over integer (in a single-valued representation) or half-odd-integer (in a double-valued one) as follows:

$\begin{align*}
A : & \quad m = 0, \\
T_1 : & \quad m = 1, 0, -1, \\
T_2 : & \quad m = 2, 0, -2, \\
G : & \quad m = 2, 1, -1, -2, \\
H : & \quad m = 2, 1, 0, -1, -2,
\end{align*}$

$\begin{align*}
E'_1 : & \quad \mu = 1/2, -1/2, \\
E'_2 : & \quad \mu = 3/2, -3/2, \\
G' : & \quad \mu = 3/2, 1/2, -1/2, -3/2, \\
I' : & \quad \mu = 5/2, 3/2, 1/2, -1/2, -3/2, -5/2,
\end{align*}$

where, as in the angular momentum theory, the subscript $\mu$ is replaced by $m$ when it is integer.

The icosahedral double group $I'_h$ is the direct product of $I'$ and the inversion group $\{E, P\}$, where $P$ is the inversion operator. According to the parity, the irreducible representations of $I'_h$ are denoted as $\Gamma_g$ (even) and $\Gamma_u$ (odd), respectively. The character table of the double group $I'_h$ was listed in Table 1 of [3]. In this note we will pay more attention to the double group $I'$.

### 3. Irreducible bases

The rank of the double group $I'$ is three. We choose $T_0$, $S_1$ and $E'$ as the generators of $I'$. 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 $I'$ such that the representation matrices of
generator $T_0$ are diagonal with the diagonal elements $\eta^\mu$. Assume that the bases $\Phi_{\mu\nu}$ in the $\Gamma$ group space are the eigenstates of left-action and right-action of $T_0$:

$$T_0 \Phi_{\mu\nu} = \eta^\mu \Phi_{\mu\nu}, \quad \Phi_{\mu\nu} T_0 = \eta^\nu \Phi_{\mu\nu},$$

(9)

where the constant $\eta$ satisfies the following equations:

$$\eta = \exp(-i2\pi/5), \quad \sum_{m=0}^{4} \eta^m = 0,$$

$$p = \eta + \eta^{-1} = (\sqrt{5} - 1)/2, \quad p^{-1} = 1 + \eta + \eta^{-1} = (\sqrt{5} + 1)/2,$$

$$q = i(\eta - \eta^{-1}) = (\sqrt{5}p^{-1})^{1/2}, \quad i(\eta^2 - \eta^{-2}) = qp.$$

(10)

The bases $\Phi_{\mu\nu}$ can be easily calculated by the projection operator $P_\mu$ (see p.113 in [4]):

$$\Phi_{\mu\nu} = c P_\mu R P_\nu, \quad P_\mu = \frac{1}{10} \sum_{a=0}^{4} \eta^{-\mu a} \left(E + \eta^{-5\mu} E'\right) T_0^a,$$

(11)

where $c$ is a normalization factor. The choice of the group element $R$ in (11) will not affect the results except for the factor $c$. The subscripts $\mu$ and $\nu$ should be integer or half-odd-integer, simultaneously. In the following we choose $E, S_{11}, S_5$ and $S_{10}$ as the group element $R$, respectively, and obtain four independent sets of bases $\Phi^{(i)}_{\mu\nu}$:

$$\Phi^{(1)}_{\mu\mu} = \frac{E + \eta^{-5\mu} E'}{\sqrt{10}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a,$$

$$\Phi^{(2)}_{\mu\mu} = \frac{E + \eta^{-5\mu} E'}{\sqrt{10}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a S_{11}$$

$$= \frac{E + \eta^{-5\mu} E'}{\sqrt{10}} \left(S_{11} + \eta^{-2\mu} S_{12} + \eta^{-4\mu} S_{13} + \eta^{-4\mu} S_{14} + \eta^{2\mu} S_{15}\right),$$
\[ \Phi^{(3)}_{\mu\nu} = \frac{E + \eta^{-5\mu} E'}{5\sqrt{2}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a S_{10} \sum_{b=0}^{4} \eta^{-\nu b} T_0^b \]
\[ = \frac{E + \eta^{-5\mu} E'}{5\sqrt{2}} \left\{ (S_{10} + \eta^{-\mu} R_5^2 + \eta^{-2\mu} T_1^4 + \eta^{2\mu} T_4 + \eta^\mu R_4) \right. \]
\[ + \eta^{(\mu-\nu)} (S_4 + \eta^{-\mu} R_5^2 + \eta^{-2\mu} T_1^4 + \eta^{2\mu} T_3 + \eta^\mu R_3) \]
\[ + \eta^{2(\mu-\nu)} (S_3 + \eta^{-\mu} R_5^2 + \eta^{-2\mu} T_1^4 + \eta^{2\mu} T_2 + \eta^\mu R_2) \]
\[ + \eta^{-2(\mu-\nu)} (S_2 + \eta^{-\mu} R_5^2 + \eta^{-2\mu} T_1^4 + \eta^{2\mu} T_1 + \eta^\mu R_1) \]
\[ \left. + \eta^{-(\mu-\nu)} (S_1 + \eta^{-\mu} R_5^2 + \eta^{-2\mu} T_1^4 + \eta^{2\mu} T_5 + \eta^\mu R_5) \right\} , \] (12)
\[ \Phi^{(4)}_{\mu\nu} = \frac{E + \eta^{-5\mu} E'}{5\sqrt{2}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a S_{10} \sum_{b=0}^{4} \eta^{-\nu b} T_0^b \]
\[ = \frac{E + \eta^{-5\mu} E'}{5\sqrt{2}} \left\{ (S_{10} + \eta^{-\mu} T_1^3 + \eta^{-2\mu} R_6^2 + \eta^{2\mu} R_9 + \eta^{\mu} T_5^2) \right. \]
\[ + \eta^{(\mu-\nu)} (S_9 + \eta^{-\mu} T_1^3 + \eta^{-2\mu} R_1^2 + \eta^{2\mu} R_8 + \eta^{\mu} T_4^3) \]
\[ + \eta^{2(\mu-\nu)} (S_8 + \eta^{-\mu} T_1^3 + \eta^{-2\mu} R_6^2 + \eta^{2\mu} R_7 + \eta^{\mu} T_3^3) \]
\[ + \eta^{-2(\mu-\nu)} (S_7 + \eta^{-\mu} T_1^3 + \eta^{-2\mu} R_6^2 + \eta^{2\mu} R_6 + \eta^{\mu} T_2^3) \]
\[ \left. + \eta^{-(\mu-\nu)} (S_6 + \eta^{-\mu} T_1^3 + \eta^{-2\mu} R_6^2 + \eta^{2\mu} R_1 + \eta^{\mu} T_1^2) \right\} . \]

where and hereafter the subscript $\overline{\mu}$ denotes $-\mu$. Those bases $\Phi^{(i)}_{\mu\nu}$ should be combined into the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ belonging to the given irreducible representation $\Gamma$. The combinations can be determined from the condition that the irreducible basis should be the eigenstate of a class operator $W$, which was called CSCO-I in [3]. The eigenvalues $\alpha_{\Gamma}$ can be calculated from the characters [3] in the irreducible representations $\Gamma$:

\[ W = \sum_{j=0}^{5} \left( T_j + E' T_j^1 \right) , \quad W \psi^{\Gamma}_{\mu\nu} = \psi^{\Gamma}_{\mu\nu} W = \alpha_{\Gamma} \psi^{\Gamma}_{\mu\nu} , \]
\[ \alpha_A = 12 , \quad \alpha_{T_1} = 4p^{-1} , \quad \alpha_{T_2} = -4p , \quad \alpha_{G} = -3 , \quad \alpha_{H} = 0 , \]
\[ \alpha_{E_1} = 6p^{-1} , \quad \alpha_{E_2'} = -6p , \quad \alpha_{G'} = 3 , \quad \alpha_{\mu'} = -2 . \] (13)

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

\[ \psi^{\Gamma}_{\mu\nu} = N^{-1/2} \sum_{i=1}^{4} c_i \Phi^{(i)}_{\mu\nu} , \] (14)

where $N$ is the normalization factor. In principle, $\psi^{\Gamma}_{\mu\nu}$ can change a phase depending on $\mu$ and $\nu$. We choose the phases such that the representation matrices of $I$ coincide with
those in the subduced representations of $D^j$ of SO(3):

$$
\begin{align*}
D^0(R) & = D^A(R), & D^1(R) & = D^{T_1}(R), & D^2(R) & = D^{H}(R), \\
D^{1/2}(R) & = D^{E_1}(R), & D^{3/2}(R) & = D^{G}(R), & D^{5/2}(R) & = D^{I}(R).
\end{align*}
$$

(15)

The representation matrices of $E'$ and $T_0$ are diagonal with the diagonal elements $\pm 1$ and $\eta^\mu$, respectively (see (9)), and those of another generator $S_1$ of I are as follows:

$$
D^A(S_1) = 1, \quad D^{T_1}(S_1) = \frac{1}{\sqrt{3}} \begin{pmatrix}
-p^{-1} & -\sqrt{2} & -p \\
-\sqrt{2} & 1 & \sqrt{2} \\
-p & \sqrt{2} & -p^{-1}
\end{pmatrix}, \\
D^{T_2}(S_1) = \frac{1}{\sqrt{3}} \begin{pmatrix}
-p & \sqrt{2} & p^{-1} \\
\sqrt{2} & -1 & \sqrt{2} \\
p^{-1} & \sqrt{2} & -p
\end{pmatrix}, \quad D^{G}(S_1) = \frac{1}{\sqrt{3}} \begin{pmatrix}
-1 & -p & -p^{-1} & 1 \\
-p & 1 & -1 & -p^{-1} \\
p^{-1} & -1 & 1 & -p \\
1 & -p^{-1} & -p & -1
\end{pmatrix}, \\
D^{H}(S_1) = \frac{1}{5} \begin{pmatrix}
p^{-2} & 2p^{-1} & \sqrt{6} & 2p & p^2 \\
2p^{-1} & p^2 & -\sqrt{6} & -p^{-2} & -2p \\
\sqrt{6} & -\sqrt{6} & -1 & \sqrt{6} & \sqrt{6} \\
2p & -p^{-2} & \sqrt{6} & p^2 & -2p^{-1} \\
p^2 & -2p & \sqrt{6} & -2p^{-1} & -p^{-2}
\end{pmatrix}, \\
D^{E_1}(S_1) = \frac{iq}{\sqrt{5}} \begin{pmatrix}
-1 & -p \\
-p & 1
\end{pmatrix}, \quad D^{E_2}(S_1) = \frac{iq}{\sqrt{5}} \begin{pmatrix}
-p & -1 \\
-1 & p
\end{pmatrix}, \\
D^{G'}(S_1) = \frac{iq}{5} \begin{pmatrix}
p^{-1} & \sqrt{3} & \sqrt{3}p & p^2 \\
\sqrt{3} & -p^2 & -p^{-1} & -\sqrt{3}p \\
\sqrt{3}p & -p^{-1} & p^2 & \sqrt{3} \\
p^2 & -\sqrt{3}p & \sqrt{3} & -p^{-1}
\end{pmatrix}, \\
D^{I'}(S_1) = \frac{iq}{5\sqrt{5}} \begin{pmatrix}
-p^{-2} & -\sqrt{5}p^{-1} & -\sqrt{10} & -\sqrt{10}p & -\sqrt{5}p^2 & -p^3 \\
-\sqrt{5}p^{-1} & -\sqrt{5}p & \sqrt{10}p & \sqrt{10} & \sqrt{5} & \sqrt{5}p^2 \\
-\sqrt{10} & \sqrt{10}p & \sqrt{5} & -\sqrt{5}p & -\sqrt{10} & -\sqrt{10}p \\
-\sqrt{10}p & \sqrt{10} & -\sqrt{5}p & -\sqrt{5} & \sqrt{10}p & \sqrt{10} \\
-\sqrt{5}p^2 & \sqrt{5} & -\sqrt{10} & \sqrt{10}p & \sqrt{5}p & -\sqrt{5}p^{-1} \\
-p^3 & \sqrt{5}p^2 & -\sqrt{10}p & \sqrt{10} & -\sqrt{5}p^{-1} & p^{-2}
\end{pmatrix}.
$$

(16)
The normalization factors $N$ and combination coefficients $c_i$ are listed in Table 1.

**Table 1**

Now, we obtain the irreducible bases $\psi_{\Gamma}^{\mu \nu}$ satisfying (1). The irreducible bases of the group $I'_h$ can be expressed as follows:

$$
\psi_{\Gamma}^{\mu \nu} = 2^{-1/2} (E + P) \psi_{\mu \nu}, \quad \psi_{\Gamma}^{\mu \nu} = 2^{-1/2} (E - P) \psi_{\mu \nu}.
$$

(17)

4. Applications to the angular momentum states

Due to the properties (1), we can obtain the irreducible function bases 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:

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

(18)

When $j$ is an integer $\ell$, $|\ell, m\rangle$ is nothing but the spherical harmonics $Y^{\ell}_{m}(\theta, \varphi)$.

From Fig.1. and (3) we have:

$$
E' |j, \mu\rangle = (-1)^{2j} |j, \mu\rangle, \quad T_0 |j, \mu\rangle = \eta^\mu |j, \mu\rangle,
$$

$$
S_5 |j, \mu\rangle = \sum_{\nu} D^j_{\nu \mu}(-\pi/5, 2\theta_4, 7\pi/5) |j, \nu\rangle = \sum_{\nu} e^{-i\nu \pi} \eta^{\mu - \nu} d^j_{\nu \mu}(2\theta_4) |j, \nu\rangle
$$

$$
S_{10} |j, \mu\rangle = \sum_{\nu} D^j_{\nu \mu}(-\pi/5, 2\theta_5, 6\pi/5) |j, \nu\rangle = \sum_{\nu} e^{i\nu \pi} \eta^{3\mu + 2\nu} d^j_{\nu \mu}(2\theta_5) |j, \nu\rangle
$$

$$
S_{11} |j, \mu\rangle = \sum_{\nu} D^j_{\nu \mu}(0, \pi, 4\pi/5) |j, \mu\rangle = (-1)^{j - \mu} \eta^{2\mu} |j, -\mu\rangle.
$$

(19)

where $d^j(\theta)$ is the usual $D$-function in the angular momentum theory [1], and

$$
\cos \theta_4 = \sin \theta_5 = q/\sqrt{5}, \quad \cos \theta_5 = \sin \theta_4 = qp/\sqrt{5}.
$$

(20)

Now, it is easy to obtain the combinations of the angular momentum states $\psi_{\mu \lambda}^{\Gamma} |j, \rho\rangle$, belonging to the $\mu$ row of the irreducible representation $\Gamma$ of $\Gamma'$:

$$
\psi_{\mu \lambda}^{\Gamma} |j, \rho\rangle = \sqrt{10/N} \delta'_{\lambda \rho} \sum_{\nu} \delta'_{\nu \mu} \left\{ c_1 \delta_{\rho \nu} + c_2 \delta_{\rho \nu}(-1)^{j - \rho} \eta^{2\rho} 
+ \sqrt{5} c_3 e^{-i\rho \eta^{j - \nu}} d^{j}_{\nu \rho}(2\theta_4) + \sqrt{5} c_4 e^{i\rho \eta^{j - \nu}} d^{j}_{\nu \rho}(2\theta_5) \right\} |j, \nu\rangle,
$$

(21)
where $N$ and $c_i$ were given in Table 1, $\delta'_{\lambda \rho}$ is defined as follows:

\[
\delta'_{\lambda \rho} = \begin{cases} 
1 & \text{when } (\lambda - \rho)/5 = \text{integer} \\
0 & \text{otherwise.}
\end{cases}
\] (22)

In driving (21) some terms were merged so that the functions need be normalized again.

(21) is our main formula. For fixed $\lambda$ and $\rho$, satisfying $\delta'_{\lambda \rho} = 1$, we obtain the combinations of the angular momentum states $\psi^\Gamma_{\mu \lambda} |j, \rho\rangle$, belonging to the $\mu$ row of the irreducible representation $\Gamma$ of $\Gamma'$. Different choice of $\lambda$ and $\rho$ may cause the combinations vanishing, dependent on each other, or independent. The number of independent combinations depends upon the number of times that the irreducible representation $\Gamma$ of $\Gamma'$ appears in the reduced form of the subduced representation of $D^j$ of SU(2). The latter is completely determined by the character of the representation and listed in Table 2 of [3].

Those combinations are very easy to be calculated by a simple computer file or even by hand. In the following we list some combinations as examples.

\[
\begin{align*}
\psi^A_{00} |0, 0\rangle &= 2\sqrt{30} |0, 0\rangle, & \psi^{T_1}_{11} |1, 1\rangle &= 2\sqrt{10} |1, \mu\rangle, \\
\psi^H_{\mu 2} |2, 2\rangle &= 2\sqrt{6} |2, \mu\rangle, & \psi^{E_i}_{\mu(1/2)} |1/2, 1/2\rangle &= -i2\sqrt{15} |1/2, \mu\rangle, \\
\psi^{G'}_{\mu(3/2)} |3/2, 3/2\rangle &= i\sqrt{30} |3/2, \mu\rangle, & \psi^{T'}_{\mu(5/2)} |5/2, 5/2\rangle &= -i2\sqrt{5} |5/2, \mu\rangle.
\end{align*}
\]

\[
\begin{align*}
\psi^{T_2}_{22} |3, 3\rangle &= -4 \left( \sqrt{3/5} |3, 2\rangle + \sqrt{2/5} |3, -3\rangle \right), \\
\psi^{T_2}_{12} |3, 3\rangle &= -4 |3, 0\rangle, \\
\psi^{T_2}_{12} |3, 3\rangle &= -4 \left( -\sqrt{2/5} |3, 3\rangle + \sqrt{3/5} |3, -2\rangle \right), \\
\psi^{G}_{22} |3, 3\rangle &= 3\sqrt{2} \left( -\sqrt{2/5} |3, 2\rangle + \sqrt{3/5} |3, -3\rangle \right), \\
\psi^{G}_{12} |3, 3\rangle &= 3\sqrt{2} |3, 1\rangle, \\
\psi^{G}_{12} |3, 3\rangle &= 3\sqrt{2} |3, -1\rangle, \\
\psi^{G}_{22} |3, 3\rangle &= 3\sqrt{2} \left( \sqrt{3/5} |3, 3\rangle + \sqrt{2/5} |3, -2\rangle \right).
\end{align*}
\]
\[
\begin{align*}
\psi_{3/2, 3/2}^{E_2} |7/2, 7/2\rangle &= -i3\sqrt{2} \left( -\sqrt{7/10} |7/2, 3/2\rangle + \sqrt{3/10} |7/2, -7/2\rangle \right), \\
\psi_{3/2, 3/2}^{E_2} |7/2, 7/2\rangle &= -i3\sqrt{2} \left( \sqrt{3/10} |7/2, 7/2\rangle + \sqrt{7/10} |7/2, -3/2\rangle \right), \\
\psi_{3/2, 3/2}^{I^\prime} |7/2, 7/2\rangle &= i\sqrt{14} \left( \sqrt{1/50} |7/2, 5/2\rangle + 7/\sqrt{50} |7/2, -5/2\rangle \right), \\
\psi_{3/2, 3/2}^{I^\prime} |7/2, 7/2\rangle &= i\sqrt{14} \left( -\sqrt{3/10} |7/2, 3/2\rangle - \sqrt{7/10} |7/2, -7/2\rangle \right), \\
\psi_{1/2, 3/2}^{I^\prime} |7/2, 7/2\rangle &= i\sqrt{14} |7/2, 1/2\rangle, \\
\psi_{1/2, 3/2}^{I^\prime} |7/2, 7/2\rangle &= -i\sqrt{14} |7/2, -1/2\rangle, \\
\psi_{3/2, 3/2}^{I^\prime} |7/2, 7/2\rangle &= i\sqrt{14} \left( -\sqrt{7/10} |7/2, 7/2\rangle + \sqrt{3/10} |7/2, -3/2\rangle \right), \\
\psi_{5/2, 3/2}^{I^\prime} |7/2, 7/2\rangle &= i\sqrt{14} \left( 7/\sqrt{50} |7/2, 5/2\rangle - 1/\sqrt{50} |7/2, -5/2\rangle \right).
\end{align*}
\]

5. Conclusion

If the Hamiltonian of a system has a given symmetry, the symmetry adapted bases are very useful in calculating the eigenvalues and eigenstates. 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 note we calculate the explicit form of the irreducible bases of $I^\prime$ group space, and obtain a general formula for calculating the combinations of angular momentum states into the irreducible basis functions belonging to the given row of a given irreducible representation of the icosahedral double group $I^\prime$. This method is effective for any double point group.

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Table 1  Irreducible bases in the group space of $\Gamma'$

$$\psi_{\mu\nu}^{\Gamma} = N^{-1/2} \sum_{i=1}^{4} c_i \Phi^{(i)}_{\mu\nu},$$

$$\eta = \exp(-i2\pi/5), \quad p = \eta + \eta^{-1}, \quad q = i(\eta - \eta^{-1}).$$

$$\psi_{00}^{A} = (\Phi^{(1)}_{00} + \Phi^{(2)}_{00} + \sqrt{5}\Phi^{(3)}_{00} + \sqrt{5}\Phi^{(4)}_{00}) / \sqrt{12}.$$

| $\Gamma = T_1$ | $\Gamma = T_2$ |
|----------------|----------------|
| $\mu$ | $\nu$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $N$ | $\mu$ | $\nu$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $N$ |
| 1 | 1 | 1 | $-p^{-1}$ | $-p$ | 4 | 2 | 2 | 1 | $-p$ | $-p^{-1}$ | 4 |
| 0 | 1 | $\eta^{-1}$ | $\eta^2$ | 2 | 0 | 2 | $\eta^{-2}$ | $\eta^{-1}$ | 2 |
| $\Upsilon$ | 1 | $\eta^{-2}$ | $-\eta^{-2}p$ | $-\eta^{-1}p^{-1}$ | 4 | $\Upsilon$ | 2 | $-\eta$ | $\eta^{-1}p$ | $\eta^{-2}p$ | 4 |
| 1 | 0 | $-\eta$ | $\eta^{-2}$ | 2 | 0 | $\eta^2$ | $-\eta$ | 2 |
| 0 | 0 | 1 | 1 | 1 | 1 | 4 | 0 | 0 | 1 | $-1$ | $-1$ | 1 | 4 |
| $\Upsilon$ | 0 | $\eta^{-1}$ | $-\eta^2$ | 2 | $\Upsilon$ | 0 | $\eta^{-2}$ | $-\eta^{-1}$ | 2 |
| 1 | $\Upsilon$ | $\eta^2$ | $-\eta^2p$ | $-\eta^{-1}p^{-1}$ | 4 | 2 | $\Upsilon$ | $-\eta^{-1}$ | $\eta^{-1}p^{-1}$ | $\eta^2p$ | 4 |
| 0 | $\Upsilon$ | $\eta$ | $-\eta^{-2}$ | 2 | $\Upsilon$ | $\eta^2$ | $-\eta$ | 2 |
| $\Upsilon$ | $\Upsilon$ | 1 | $-p^{-1}$ | $-p$ | 4 | $\Upsilon$ | 1 | $-p$ | $-p^{-1}$ | 4 |

| $\Gamma = G$ |
|----------------|
| $\mu$ | $\nu$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $N$ | $\mu$ | $\nu$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $N$ |
| 2 | 2 | 1 | $-1$ | $1$ | 3 | 2 | $\Upsilon$ | $-\eta^{-2}p^{-1}$ | $-\eta^{-1}p$ | 3 |
| 1 | 2 | $-\eta^{-1}p$ | $-\eta^2p^{-1}$ | 3 | 1 | $\Upsilon$ | $\eta^2$ | $-\eta^2$ | $\eta$ | 3 |
| $\Upsilon$ | 2 | $-\eta^2p^{-1}$ | $-\eta p$ | 3 | $\Upsilon$ | 1 | 1 | $-1$ | 3 |
| $\Upsilon$ | 2 | $\eta$ | $\eta$ | $-\eta^{-2}$ | 3 | $\Upsilon$ | $-\eta^{-1}p$ | $-\eta^{-2}p^{-1}$ | 3 |
| 2 | 1 | $-\eta p$ | $-\eta^{-2}p^{-1}$ | 3 | 2 | $\Upsilon$ | $\eta^{-1}$ | $\eta^{-1}$ | $-\eta^2$ | 3 |
| 1 | 1 | 1 | $1$ | $-1$ | 3 | 1 | $\Upsilon$ | $-\eta^{-2}p^{-1}$ | $-\eta^{-1}p$ | 3 |
| $\Upsilon$ | 1 | $\eta^{-2}$ | $-\eta^{-2}$ | $\eta^{-1}$ | 3 | $\Upsilon$ | $\eta^{-1}$ | $-\eta^{-2}p^{-1}$ | $\eta^{-2}$ | 3 |
| $\Upsilon$ | 1 | $-\eta^2p^{-1}$ | $-\eta p$ | 3 | $\Upsilon$ | 1 | $-1$ | 3 |

| $\Gamma = H$ |
|----------------|
| $\mu$ | $\nu$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $N$ | $\mu$ | $\nu$ | $c_1$ | $c_2$ | $c_3$ | $c_4$ | $N$ |
| 2 | 2 | $\sqrt{5}$ | $p^2$ | $p^2$ | 12 | $\Upsilon$ | 0 | $\eta^{-1}$ | $\eta^2$ | 2 |
| 1 | 2 | $\eta^{-1}p^{-1}$ | $-\eta^2p$ | 3 | $\Upsilon$ | 0 | $\eta^{-2}$ | $\eta^{-1}$ | 2 |
| 0 | 2 | $\eta^{-2}$ | $\eta^{-1}$ | 2 | $\Upsilon$ | $\eta^{-2}p$ | $-\eta^{-1}p^{-1}$ | 3 |
| $\Upsilon$ | 2 | $\eta^2p$ | $-\eta^{-1}p^{-1}$ | 3 | 1 | $\Upsilon$ | $-\sqrt{5}\eta^2$ | $-\eta^2p^{-2}$ | $-\eta p^2$ | 12 |
| $\Upsilon$ | 2 | $\sqrt{5}\eta$ | $\eta p^2$ | $\eta^{-2}p^{-2}$ | 12 | 0 | $\Upsilon$ | $\eta$ | $\eta^{-2}$ | 2 |
| 2 | 1 | $\eta p^{-1}$ | $-\eta^{-2}p^{-1}$ | 3 | $\Upsilon$ | $\sqrt{5}$ | $p^2$ | $p^2$ | 12 |
| 1 | 1 | $\sqrt{5}$ | $p^2$ | $p^{-2}$ | 12 | $\Upsilon$ | $\sqrt{5}$ | $-\eta^{-1}p^{-1}$ | $\eta^2p$ | 3 |
| 0 | 1 | $-\eta^{-1}$ | $-\eta^2$ | 2 | 2 | $\Upsilon$ | $\sqrt{5}\eta^{-1}$ | $\eta^{-1}p^{-1}$ | $\eta^2p^{-2}$ | 12 |
| $\Upsilon$ | 1 | $-\sqrt{5}\eta^{-2}$ | $-\eta^{-2}p^{-2}$ | $-\eta^{-1}p^2$ | 12 | 1 | $\Upsilon$ | $-\eta^{-2}p$ | $\eta^{-1}p^{-1}$ | 3 |
| $\Upsilon$ | 1 | $-\eta^2p$ | $\eta^{-1}p^{-1}$ | 3 | 0 | $\Upsilon$ | $\eta^2$ | $\eta$ | 2 |
| 2 | 0 | $\eta^2$ | $\eta$ | 2 | $\Upsilon$ | $\eta p^{-1}$ | $\eta^{-2}p$ | 3 |
| 1 | 0 | $-\eta$ | $-\eta^{-2}$ | 2 | 2 | $\Upsilon$ | $\sqrt{5}$ | $p^{-2}$ | $p^2$ | 12 |
| 0 | 0 | $\sqrt{5}$ | $\sqrt{5}$ | $-1$ | $-1$ | 12 | 12 |
\[
\begin{array}{cccccccc}
\Gamma = E'_1 & & & & & & & \\
\begin{array}{cccccc}
2\mu & 2\nu & c_1 & c_2 & c_3 & c_4 & N \\
1 & 1 & -i & q & qp & 6 \\
\text{T} & 1 & -i\eta^{-1} & \eta^{-1}qp & -\eta^2q & 6 \\
1 & \text{T} & i\eta & \eta qp & -\eta^{-2}q & 6 \\
\text{T} & \text{T} & -i & -q & -qp & 6 \\
\end{array}
\end{array}
\]

\[
\begin{array}{cccccccc}
\Gamma = E'_2 & & & & & & & \\
\begin{array}{cccccc}
2\mu & 2\nu & c_1 & c_2 & c_3 & c_4 & N \\
3 & 3 & -i & qp & -q & 6 \\
\text{T} & 3 & i\eta^2 & \eta^2q & \eta qp & 6 \\
3 & \text{T} & -i\eta^{-2} & \eta^{-2}q & \eta^{-1}qp & 6 \\
3 & \text{T} & -i & -qp & q & 6 \\
\end{array}
\end{array}
\]

\[
\begin{array}{cccccccc}
\Gamma = G' & & & & & & & \\
\begin{array}{cccccc}
2\mu & 2\nu & c_1 & c_2 & c_3 & c_4 & N \\
3 & 3 & i\sqrt{5} & qp^{-1} & qp^2 & 15 \\
1 & 3 & \eta^{-1}q & -\eta^2qp & 5 \\
\text{T} & 3 & \eta^{-2}qp & \eta^{-1}q & 5 \\
3 & \text{T} & i\sqrt{5}q^2 & \eta^2q^2 & -\eta qp^{-1} & 15 \\
3 & 1 & \eta q & -\eta^{-2}qp & 5 \\
1 & 1 & i\sqrt{5} & -qp^2 & qp^{-1} & 15 \\
\text{T} & 1 & -i\sqrt{5}q^{-1} & -\eta^{-1}qp^{-1} & -\eta^2qp^2 & 15 \\
3 & 1 & -\eta^{-2}qp & -\eta^{-1}q & 5 \\
\end{array}
\end{array}
\]

\[
\begin{array}{cccccccc}
\Gamma = I' & & & & & & & \\
\begin{array}{cccccc}
2\mu & 2\nu & c_1 & c_2 & c_3 & c_4 & N \\
5 & 5 & -i5 & qp^{-2} & qp^3 & 50 \\
3 & 5 & \eta^{-1}qp^{-1} & -\eta^2qp^2 & 10 \\
1 & 5 & \eta^{-2}q & \eta^{-1}qp & 5 \\
\text{T} & 5 & \eta^2qp & \eta q & 5 \\
3 & 5 & \eta qp^2 & \eta^{-2}qp^{-1} & 10 \\
5 & 5 & -i5 & qp^3 & -qp^{-2} & 50 \\
3 & 3 & \eta^2q & \eta^2qp & 10 \\
1 & 3 & -\eta^{-1}qp & -\eta^2q & 5 \\
\text{T} & 3 & -\eta^{-2}q & \eta^1qp & 5 \\
3 & \text{T} & i\sqrt{5}q^2 & -\eta^2q & \eta qp & 10 \\
5 & 3 & -\etaqp^2 & -\eta^{-2}qp^{-1} & 10 \\
5 & 1 & \eta^2q & \eta qp & 5 \\
1 & 1 & -\etaqp & -\eta q & 10 \\
\text{T} & 1 & -\eta\sqrt{5}q^{-1} & \eta^{-1}qp & \eta^2q & 10 \\
3 & 1 & \eta^{-2}q & -\eta^{-1}qp & 5 \\
5 & 1 & \eta^2q & \eta qp & 5 \\
\text{T} & 1 & -i5 & -qp^2 & -qp^{-3} & 50 \\
\end{array}
\end{array}
\]

\[
\Gamma = \Gamma' & & & & & & & \\
\begin{array}{cccccccc}
\end{array}
\]

\[
\begin{array}{cccccccc}
\text{G} & & & & & & & \\
\end{array}
\]