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Correlations of Spin States for Icosahedral Double Group

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The irreducible bases of the icosahedral double groups $\mathbf{I}'$ and $\mathbf{I}'_h$ are explicitly presented in their respective group spaces. Applying these bases to the spin states $|j, \mu\rangle$, we obtain a simple formula for combining the spin states into the symmetry-adapted bases which belong to a given row of given irreducible representations of $\mathbf{I}'$ and $\mathbf{I}'_h$.

1. INTRODUCTION

Metallo-fullerene is a kind of fullerene cage with a metal atom or atoms in the center of the cage. The study of the metallo-fullerene has attracted considerable attention from physicists and chemists since Heath *et al.* [12] showed that metal-containing fullerene could be generated. To classify its electronic states in the case of spin–orbit coupling, especially for electronic states with half-integer spin, one has to study the double group symmetry [2].

Recently, the character table and the correlation tables related to $\mathbf{I}'_h$ have been presented by Balasubramanian [1]. The correlation tables can be obtained from the character table using standard group-theoretical methods [11]. From the correlation tables, states with a low angular momentum can be combined by a similarity transformation into a state belonging to a given row of a given irreducible representation of $\mathbf{I}'$. However, this becomes a tedious task as the angular momentum is increased. Fortunately, the difficulty can be overcome by using the irreducible bases in the group space of $\mathbf{I}'$. In the

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present work, we present a simple formula [see below (21)] to combine the spin states into symmetry-adapted bases which belong to a given row of given irreducible representations of $\mathbf{I}'$ and $\mathbf{I}'_h$. Irreducible bases in the group space of $\mathbf{I}'$ and combinations of the spin states are frequently used to study vibrational and rotational problems in C_{60} [7].

From the viewpoint of group theory (ref. 11, p. 106), the group element R plays the role of a basis in the group space, which is the representation space of the regular representation. The number of times that each irreducible representation is contained in the regular representation is equal to the dimension of the representation. One can obtain the new bases $\psi^{\Gamma}_{\mu\nu}$ belonging to the μ (ν) row of the irreducible representation Γ in the left (right) action of a group element by reducing the regular representation

$$R\psi^{\Gamma}_{\mu\nu} = \sum_{\rho} \psi^{\Gamma}_{\rho\nu} D^{\Gamma}_{\rho\mu}(R), \qquad \psi^{\Gamma}_{\mu\nu} R = \sum_{\rho} D^{\Gamma}_{\nu\rho}(R)\psi^{\Gamma}_{\mu\rho} \tag{1}$$

where $\psi^{\Gamma}_{\mu\nu}$ 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 nonvanishing angular momentum states $|j,\rho\rangle$, one can obtain the combinations $\psi^{\Gamma}_{\mu\nu}|j, \rho\rangle$, which belong to the μ row of the representation Γ of the point group G,

$$R\psi^{\Gamma}_{\mu\nu}|j, \rho\rangle = \sum_{\tau} D^{\lambda}_{\tau\mu}(R)\psi^{\lambda}_{\tau\nu}|j, \rho\rangle \tag{2}$$

This method is effective for the study of both integer and half-integer angular momentum states. The purpose of this paper is to obtain the irreducible bases of the group space and give a simple formula for combining the spin states into symmetry-adapted bases by applying those irreducible bases to the spin states $|j, \mu\rangle$. This paper is based on our previous work [8–10].

2. ICOSAHEDRAL DOUBLE GROUP

As shown in Fig. 1, the upper vertices of the icosahedron are labeled by A_j and their opposite vertices by B_j ($0 \le j \le 5$). The z and y axes point from the center O to A_0 and the midpoint of A_2B_5, respectively.

The icosahedral group $\mathbf{I}$ has 6 fivefold axes, 10 threefold axes, and 15 twofold axes. One of the fivefold axes is along the z axis, and the rest point from B_j to A_j ($1 \le j \le 5$) with polar angle θ_1 and azimuthal angles $\varphi^{(1)}_j$. Rotations through $2\pi/5$ around those fivefold axes are denoted by T_j ($0 \le j \le 5$). The threefold axes join the centers of two opposite faces. The polar angles of the first and last five axes are θ_2, and θ_3, respectively, and the azimuthal angles are $\varphi^{(2)}_j$. Rotations through $2\pi/3$ around those threefold axes are denoted by R_j ($1 \le j \le 10$). The twofold axes join the midpoints of two

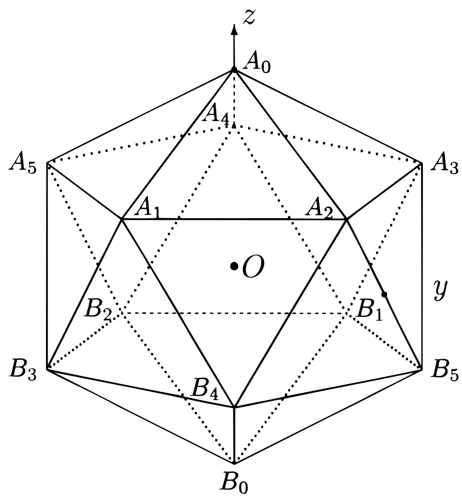

Fig. 1. Icosahedron with $\mathbf{I}_h$ symmetry.

opposite edges. The polar and azimuthal angles of the first, next, and last five axes are θ_4, $\varphi_j^{(1)}$, θ_5 and $\varphi_j^{(2)}$, π, and $\varphi_j^{(3)}$, respectively. Rotations through π around those twofold axes are denoted by S_j $(1 \le j \le 15)$. The angles θ_i and $\varphi_j^{(i)}$ are expressed as

$$\begin{aligned} &\tan\theta_1 = 2, && \tan\theta_2 = 3 - \sqrt{5}, && \tan\theta_3 = 3 + \sqrt{5} \\ &\tan\theta_4 = (\sqrt{5} - 1)/2, && \tan\theta_5 = (\sqrt{5} + 1)/2, && \\ &\varphi_j^{(1)} = 2(j-1)\pi/5, && \varphi_j^{(2)} = (2j-1)\pi/5, && \varphi_j^{(3)} = (4j-3)\pi/10 \end{aligned} \tag{3}$$

$SU(2)$ is the covering group of $SO(3)$ and provides the double-valued representations of $SO(3)$. To classify angular momentum states with half-integer spin, one has to extend the point group to the double point group, following the homomorphism of $SU(2)$ onto $SO(3)$,

$$\pm u(\hat{\mathbf{n}}, \omega) \rightarrow R(\hat{\mathbf{n}}, \omega) \tag{4}$$

For $SO(3)$, a rotation through 2π is equal to identity E, but it is different from identity E' of $SU(2)$,

$$R(\hat{\mathbf{n}}, 2\pi) = E, \qquad u(\hat{\mathbf{n}}, 2\pi) \equiv E' = -\mathbf{1} \tag{5}$$

Similarly, a point group G is extended into a double point group G' by introducing a new element E' with the properties

$$RE' = E'R, \qquad (E')^2 = E, \qquad R \in G \subset G', \qquad E'R \in G' \tag{6}$$

G is a subgroup of $SO(3)$, and G' is that of $SU(2)$. For definiteness, we restrict the rotation angle ω to be not larger than π

$$\begin{aligned} &R(\hat{\mathbf{n}}, \omega) \to u(\hat{\mathbf{n}}, \omega) \\ &R(\hat{\mathbf{n}}, \omega - 2\pi) = R(-\hat{\mathbf{n}}, 2\pi - \omega) \to u(-\hat{\mathbf{n}}, 2\pi - \omega) = -u(\hat{\mathbf{n}}, \omega) \\ &0 \leq \omega \leq \pi \end{aligned} \tag{7}$$

The period of ω for $SU(2)$ is 4π. The element E' is denoted by R in refs. 1 and 11 and by θ in refs. 3–6, 13, 14 and G' is denoted by $G^{\dagger}$ in refs. 3–6, 13, 14.

The $\mathbf{I}'$ contains 120 elements and nine classes. There are nine inequivalent irreducible representations for $\mathbf{I}'$: five representations A, T_1, T_2, G, and H are called single-valued, and four representations E_1', E_2', G', and I' are double-valued. The row (column) index runs over integers (in a single-valued representation) or half-integers (in a double-valued one) as follows:

$$\begin{array}{llll} A: & m = 0 & E_1': & \mu = 1/2, -1/2 \\ T_1: & m = 1, 0, -1 & E_2': & \mu = 3/2, -3/2 \\ T_2: & m = 2, 0, -2 & G': & \mu = 3/2, 1/2, -1/2, -3/2 \\ G: & m = 2, 1, -1, -2 & I': & \mu = 5/2, 3/2, 1/2, -1/2, -3/2, -5/2 \\ H: & m = 2, 1, 0, -1, -2 & & \end{array} \tag{8}$$

where the subscript μ is replaced by m when it is an integer, as in angular momentum theory.

Actually, the group $\mathbf{I}_h'$ is the direct product of $\mathbf{I}'$ and the inversion group $\{E, P\}$, where P is the inversion operator. According to the parity, the irreducible representations of $\mathbf{I}_h'$ are denoted as Γ_g (even) and Γ_u (odd), respectively. The character table of the double group $\mathbf{I}_h'$ is listed in Table 1 of ref. 1. In this work, we pay more attention to the icosahedral double group $\mathbf{I}'$, which is studied in the following section.

3. IRREDUCIBLE BASES

The rank of $\mathbf{I}'$ is three. One can choose T_0, S_1, and E' as the generators of $\mathbf{I}'$. The representation matrix of E' is equal to the unit matrix $\mathbf{1}$ in the single-valued irreducible representation and $-\mathbf{1}$ in the double-valued one. It is convenient to choose the bases in an irreducible representations of $\mathbf{I}'$ such that the representation matrices of the generator T_0 are diagonal with diagonal elements η^{μ}. In the $\mathbf{I}'$ group space, assume that the bases $\Phi_{\mu\nu}$ are the eigenstates of left action and right action of T_0,

$$T_0\Phi_{\mu\nu} = \eta^{\mu}\Phi_{\mu\nu}, \qquad \Phi_{\mu\nu}T_0 = \eta^{\nu}\Phi_{\mu\nu} \tag{9}$$

where the constant η satisfies the equations

$$\eta = \exp(-i2\pi/5), \qquad \sum_{m=0}^{4} \eta^m = 0$$
$$p = \eta + \eta^{-1} = (\sqrt{5} - 1)/2, \qquad p^{-1} = 1 + \eta + \eta^{-1} = (\sqrt{5} + 1)/2 \quad (10)$$
$$q = i(\eta - \eta^{-1}) = (\sqrt{5}p^{-1})^{1/2}, \qquad i(\eta^2 - \eta^{-2}) = qp$$

The bases $\Phi_{\mu\nu}$ can be readily obtained by the projection operator P_μ (ref 11, p. 113)

$$\Phi_{\mu\nu} = cP_\mu RP_\nu, \qquad P_\mu = \frac{1}{10}\sum_{a=0}^{4} \eta^{-\mu a}(E + \eta^{-5\mu} E')T_0^a \tag{11}$$

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 μ and ν should be both integer or both half-integer. In the following, one can choose E, S_{11}, S_5, or S_{10} as the group element R and obtain four independent sets of bases $\Phi_{\mu\nu}^{(i)}$:

$$\Phi_{\mu\mu}^{(1)} = \frac{E + \eta^{-5\mu} E'}{\sqrt{10}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a$$
$$\Phi_{\mu\mu}^{(2)} = \frac{E + \eta^{-5\mu} E'}{\sqrt{10}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a S_{11}$$
$$= \frac{E + \eta^{-5\mu} E'}{\sqrt{10}} (S_{11} + \eta^{-2\mu}S_{12} + \eta^{-4\mu}S_{13} + \eta^{4\mu}S_{14} + \eta^{2\mu}S_{15})$$
$$\Phi_{\mu\nu}^{(3)} = \frac{E + \eta^{-5\mu}E'}{5\sqrt{2}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a S_5 \sum_{b=0}^{4} \eta^{-\nu b} T_0^b \tag{12}$$
$$= \frac{E + \eta^{-5\mu}E'}{5\sqrt{2}} \{(S_5 + \eta^{-\mu}R_5^2 + \eta^{-2\mu}T_1^4 + \eta^{2\mu}T_4 + \eta^{\mu}R_4)$$
$$+ \eta^{(\mu-\nu)}(S_4 + \eta^{-\mu}R_4^2 + \eta^{-2\mu}T_5^4 + \eta^{2\mu}T_3 + \eta^{\mu}R_3)$$
$$+ \eta^{2(\mu-\nu)}(S_3 + \eta^{-\mu}R_3^2 + \eta^{-2\mu}T_4^4 + \eta^{2\mu}T_2 + \eta^{\mu}R_2)$$
$$+ \eta^{-2(\mu-\nu)}(S_2 + \eta^{-\mu}R_2^2 + \eta^{-2\mu}T_3^4 + \eta^{2\mu}T_1 + \eta^{\mu}R_1)$$
$$+ \eta^{-(\mu-\nu)}(S_1 + \eta^{-\mu}R_1^2 + \eta^{-2\mu}T_2^4 + \eta^{2\mu}T_5 + \eta^{\mu}R_5)\}$$
$$\Phi_{\mu\nu}^{(4)} = \frac{E + \eta^{-5\mu}E'}{5\sqrt{2}} \sum_{a=0}^{4} \eta^{-\mu a} T_0^a S_{10} \sum_{b=0}^{4} \eta^{-\nu b} T_0^b$$
$$= \frac{E + \eta^{-5\mu}E'}{5\sqrt{2}} \{(S_{10} + \eta^{-\mu}T_1^3 + \eta^{-2\mu}R_6^2 + \eta^{2\mu}R_9 + \eta^{\mu}T_5^2)$$

$$+ \eta^{(\mu-\nu)}(S_9 + \eta^{-\mu}T_5^3 + \eta^{-2\mu}R_{10}^2 + \eta^{2\mu}R_8 + \eta^{\mu}T_4^2)$$
$$+ \eta^{2(\mu-\nu)}(S_8 + \eta^{-\mu}T_4^3 + \eta^{-2\mu}R_9^2 + \eta^{2\mu}R_7 + \eta^{\mu}T_3^2)$$
$$+ \eta^{-2(\mu-\nu)}(S_7 + \eta^{-\mu}T_3^3 + \eta^{-2\mu}R_8^2 + \eta^{2\mu}R_6 + \eta^{\mu}T_2^2)$$
$$+ \eta^{-(\mu-\nu)}(S_6 + \eta^{-\mu}T_2^3 + \eta^{-2\mu}R_7^2 + \eta^{2\mu}R_{10} + \eta^{\mu}T_1^2))\}$$

where here and hereafter the subscript $\overline{\mu}$ denotes $-\mu$. The bases $\Phi_{\mu\nu}^{(i)}$ can be combined into irreducible bases $\psi_{\mu\nu}^{\Gamma}$ belonging to the given irreducible that the irreducible basis should be the eigenstate of a class operator W, which is called CSCO-I in refs. 3–6, 13, 14. The eigenvalues α_Γ can be obtained by the characters given by the irreducible representations Γ [1]

$$W = \sum_{j=0}^{5} (T_j + E'T_j^4), \qquad W\psi_{\mu\nu}^{\Gamma} = \psi_{\mu\nu}^{\Gamma} W = \alpha_\Gamma \psi_{\mu\nu}^{\Gamma}$$
$$\alpha_A = 12, \qquad \alpha_{T_1} = 4p^{-1}, \qquad \alpha_{T_2} = -4p, \qquad \alpha_G = -3, \qquad \alpha_H = 0 \qquad (13)$$
$$\alpha_{E_1'} = 6p^{-1}, \qquad \alpha_{E_2'} = -6p, \qquad \alpha_{G'} = 3, \qquad \alpha_{I'} = -2$$

We now calculate the matrix expression of W under the bases $\Phi_{\mu\nu}^{(i)}$ and diagonalize it.The $\psi_{\mu\nu}^{\Gamma}$ are nothing but the eigenvectors of the matrix expression of W,

$$\psi_{\mu\nu}^{\Gamma} = N^{-1/2} \sum_{i=1}^{4} c_i \Phi_{\mu\nu}^{(i)} \qquad (14)$$

where N is the normalization factor. In principle, the $\psi_{\mu\nu}^{\Gamma}$ can change the phase, depending on μ and ν. One can choose the phases to make the representation matrices of $\mathbf{I}'$ coincide with those in the subduced representations of D^j of $SO(3)$,

$$D^0(R) = D^A(R), \qquad D^1(R) = D^{T_1}(R), \qquad D^2(R) = D^H(R) \qquad (15)$$
$$D^{1/2}(R) = D^{E_1'}(R), \qquad D^{3/2}(R) = D^{G'}(R), \qquad D^{5/2}(R) = D^{I'}(R)$$

The representation matrices of E' and T_0 are diagonal, with the diagonal elements ± 1 and η^μ, respectively, and those of another generator S_1 of $\mathbf{I}'$ are written as

$$D^A(S_1) = 1$$
$$D^{T_1}(S_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} -p^{-1} & -\sqrt{2} & -p \\ -\sqrt{2} & 1 & \sqrt{2} \\ -p & \sqrt{2} & -p^{-1} \end{pmatrix}$$

$$
\begin{aligned}
D^{T_2}(S_1) &= \frac{1}{\sqrt{5}}\begin{pmatrix} -p & \sqrt{2} & p^{-1} \\ \sqrt{2} & -1 & \sqrt{2} \\ p^{-1} & \sqrt{2} & -p \end{pmatrix} \\
D^{G}(S_1) &= \frac{1}{\sqrt{5}}\begin{pmatrix} -1 & -p & -p^{-1} & 1 \\ -p & 1 & -1 & -p^{-1} \\ -p^{-1} & -1 & 1 & -p \\ 1 & -p^{-1} & -p & -1 \end{pmatrix} \\
D^{H}(S_1) &= \frac{1}{5}\begin{pmatrix} p^{-2} & 2p^{-1} & \sqrt{6} & 2p & p^2 \\ 2p^{-1} & p^2 & -\sqrt{6} & -p^{-2} & -2p \\ \sqrt{6} & -\sqrt{6} & -1 & \sqrt{6} & \sqrt{6} \\ 2p & -p^{-2} & \sqrt{6} & p^2 & -2p^{-1} \\ p^2 & -2p & \sqrt{6} & -2p^{-1} & p^{-2} \end{pmatrix} \qquad (16) \\
D^{E_1'}(S_1) &= \frac{iq}{\sqrt{5}}\begin{pmatrix} -1 & -p \\ -p & 1 \end{pmatrix} \\
D^{E_2'}(S_1) &= \frac{iq}{\sqrt{5}}\begin{pmatrix} -p & -1 \\ -1 & p \end{pmatrix} \\
D^{G'}(S_1) &= \frac{iq}{5}\begin{pmatrix} p^{-1} & \sqrt{3} & \sqrt{3}p & p^2 \\ \sqrt{3} & -p^2 & -p^{-1} & -\sqrt{3}p \\ \sqrt{3}p & -p^{-1} & p^2 & \sqrt{3} \\ p^2 & -\sqrt{3}p & \sqrt{3} & -p^{-1} \end{pmatrix} \\
D^{I'}(S_1) &= \frac{iq}{5\sqrt{5}}\begin{pmatrix} -p^{-2} & -\sqrt{5}p^{-1} & -\sqrt{10} & -\sqrt{10}p & -\sqrt{5}p^2 & -p^3 \\ -\sqrt{5}p^{-1} & -\sqrt{5}p & \sqrt{10}p & \sqrt{10} & \sqrt{5} & \sqrt{5}p^2 \\ -\sqrt{10} & \sqrt{10}p & \sqrt{5} & -\sqrt{5}p & -\sqrt{10} & -\sqrt{10}p \\ -\sqrt{10}p & \sqrt{10} & -\sqrt{5}p & -\sqrt{5} & \sqrt{10}p & \sqrt{10} \\ -\sqrt{5}p^2 & \sqrt{5} & -\sqrt{10} & \sqrt{10}p & \sqrt{5}p & -\sqrt{5}p^{-1} \\ -p^3 & \sqrt{5}p^2 & -\sqrt{10}p & \sqrt{10} & -\sqrt{5}p^{-1} & p^{-2} \end{pmatrix}
\end{aligned}
$$

The normalization factors N and combination coefficients c_i are listed in Table I.

We now obtain the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ satisfying (1). Since $\mathbf{I}_h'$ is the direct product of $\mathbf{I}'$ and the inversion group $\{E, P\}$, the irreducible bases of $\mathbf{I}_h'$ can be expressed as follows:

Table I. Irreducible Bases in the Group Space of I′

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

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

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

$\Gamma = T_1$							$\Gamma = T_2$						
μ	ν	c_1	c_2	c_3	c_4	N	μ	ν	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			$-\eta^{-1}$	η^2	2	0	2			η^{-2}	$-\eta^{-1}$	2
$\bar{1}$	1		η^{-2}	$\eta^{-2}p$	$-\eta^{-1}p^{-1}$	4	$\bar{2}$	2		$-\eta$	ηp^{-1}	$\eta^{-2}p$	4
1	0			$-\eta$	η^{-2}	2	2	0			η^2	$-\eta$	2
0	0	1	-1	1	-1	4	0	0	1	-1	-1	1	4
$\bar{1}$	0			η^{-1}	$-\eta^2$	2	$\bar{2}$	0			η^{-2}	$-\eta^{-1}$	2
1	$\bar{1}$		η^2	$-\eta^2 p$	$-\eta p^{-1}$	4	2	$\bar{2}$		$-\eta^{-1}$	$\eta^{-1}p^{-1}$	$\eta^2 p$	4
0	$\bar{1}$			η	$-\eta^{-2}$	2	0	$\bar{2}$			η^2	$-\eta$	2
$\bar{1}$	$\bar{1}$	1		$-p^{-1}$	$-p$	4	$\bar{2}$	$\bar{2}$	1		$-p$	$-p^{-1}$	4

$\Gamma = G$							$\Gamma = G$						
μ	ν	c_1	c_2	c_3	c_4	N	μ	ν	c_1	c_2	c_3	c_4	N
2	2	1		-1	1	3	2	$\bar{1}$			$-\eta^{-2}p^{-1}$	$-\eta^{-1}p$	3
1	2			$-\eta^{-1}p$	$-\eta^2 p^{-1}$	3	1	$\bar{1}$		η^2	$-\eta^2$	η	3
$\bar{1}$	2			$-\eta^2 p^{-1}$	$-\eta p$	3	$\bar{1}$	$\bar{1}$	1		1	-1	3
$\bar{2}$	2		η	η	$-\eta^{-2}$	3	$\bar{2}$	$\bar{1}$			$-\eta^{-1}p$	$-\eta^2 p^{-1}$	3
2	1			$-\eta p$	$-\eta^{-2}p^{-1}$	3	2	$\bar{2}$		η^{-1}	η^{-1}	$-\eta^2$	3
1	1	1		1	-1	3	1	$\bar{2}$			$-\eta^{-2}p^{-1}$	$-\eta^{-1}p$	3
$\bar{1}$	1		η^{-2}	$-\eta^{-2}$	η^{-1}	3	$\bar{1}$	$\bar{2}$			$-\eta p$	$-\eta^{-2}p^{-1}$	3
$\bar{2}$	1			$-\eta^2 p^{-1}$	$-\eta p$	3	$\bar{2}$	$\bar{2}$	1		-1	1	3

$\Gamma = H$							$\Gamma = H$						
μ	ν	c_1	c_2	c_3	c_4	N	μ	ν	c_1	c_2	c_3	c_4	N
2	2	$\sqrt{5}$		p^{-2}	p^2	12	$\bar{1}$	0			η^{-1}	η^2	2
1	2			$\eta^{-1}p^{-1}$	$-\eta^2 p$	3	$\bar{2}$	0			η^{-2}	η^{-1}	2
0	2			η^{-2}	η^{-1}	2	2	$\bar{1}$			$\eta^{-2}p$	$-\eta^{-1}p^{-1}$	3
$\bar{1}$	2			$\eta^2 p$	$-\eta p^{-1}$	3	1	$\bar{1}$		$-\sqrt{5}\eta^2$	$-\eta^2 p^{-2}$	$-\eta p^2$	12
$\bar{2}$	2		$\sqrt{5}\eta$	ηp^2	$\eta^{-2}p^{-2}$	12	0	$\bar{1}$			η	η^{-2}	2
2	1			ηp^{-1}	$-\eta^{-2}p$	3	$\bar{1}$	$\bar{1}$	$\sqrt{5}$		p^2	p^{-2}	12
1	1	$\sqrt{5}$		p^2	p^{-2}	12	$\bar{2}$	$\bar{1}$			$-\eta^{-1}p^{-1}$	$\eta^2 p$	3
0	1			$-\eta^{-1}$	$-\eta^2$	2	2	$\bar{2}$		$\sqrt{5}\eta^{-1}$	$\eta^{-1}p^2$	$\eta^2 p^{-2}$	12
$\bar{1}$	1		$-\sqrt{5}\eta^{-2}$	$-\eta^{-2}p^{-2}$	$-\eta^{-1}p^2$	12	1	$\bar{2}$			$-\eta^{-2}p$	$\eta^{-1}p^{-1}$	3
$\bar{2}$	1			$-\eta^2 p$	ηp^{-1}	3	0	$\bar{2}$			η^2	η	2
2	0			η^2	η	2	$\bar{1}$	$\bar{2}$			$-\eta p^{-1}$	$\eta^{-2}p$	3
1	0			$-\eta$	$-\eta^{-2}$	2	$\bar{2}$	$\bar{2}$	$\sqrt{5}$		p^{-2}	p^2	12
0	0	$\sqrt{5}$	$\sqrt{5}$	-1	-1	12							

Table I. Continued

$\Gamma = E_1'$							$\Gamma = E_2'$						
2μ	2ν	c_1	c_2	c_3	c_4	N	2μ	2ν	c_1	c_2	c_3	c_4	N
1	1	$-i$		q	qp	6	3	3	$-i$		qp	$-q$	6
$\bar{1}$	1		$-i\eta^{-1}$	$\eta^{-1}qp$	$-\eta^2 q$	6	$\bar{3}$	3		$i\eta^2$	$\eta^2 q$	ηqp	6
1	$\bar{1}$		$i\eta$	ηqp	$-\eta^{-2}q$	6	3	$\bar{3}$		$-i\eta^{-2}$	$\eta^{-2}q$	$\eta^{-1}qp$	6
$\bar{1}$	$\bar{1}$	$-i$		$-q$	$-qp$	6	$\bar{3}$	$\bar{3}$	$-i$		$-qp$	q	6

$\Gamma = G'$							$\Gamma = G'$						
2μ	2ν	c_1	c_2	c_3	c_4	N	2μ	2ν	c_1	c_2	c_3	c_4	N
3	3	$i\sqrt{5}$		qp^{-1}	qp^2	15	3	$\bar{1}$			$\eta^2 qp$	ηq	5
1	3			$\eta^{-1}q$	$-\eta^2 qp$	5	1	$\bar{1}$		$i\sqrt{5}\eta$	$-\eta qp^{-1}$	$-\eta^{-2}qp^2$	15
$\bar{1}$	3			$\eta^{-2}qp$	$\eta^{-2}q$	5	$\bar{1}$	$\bar{1}$	$i\sqrt{5}$		qp^2	$-qp^{-1}$	15
$\bar{3}$	3		$i\sqrt{5}\eta^2$	$\eta^2 qp^2$	$-\eta qp^{-1}$	15	$\bar{3}$	$\bar{1}$			$\eta^{-1}q$	$-\eta^2 qp$	5
3	1			ηq	$-\eta^{-2}qp$	5	3	$\bar{3}$		$-i\sqrt{5}\eta^{-2}$	$\eta^{-2}qp^2$	$-\eta^{-1}qp^{-1}$	15
1	1	$i\sqrt{5}$		$-qp^2$	qp^{-1}	15	1	$\bar{3}$			$-\eta^2 qp$	$-\eta q$	5
$\bar{1}$	1		$-i\sqrt{5}\eta^{-1}$	$-\eta^{-1}qp^{-1}$	$-\eta^2 qp^2$	15	$\bar{1}$	$\bar{3}$			ηq	$-\eta^{-2}qp$	5
$\bar{3}$	1			$-\eta^{-2}qp$	$-\eta^{-1}q$	5	$\bar{3}$	$\bar{3}$	$i\sqrt{5}$		$-qp^{-1}$	$-qp^2$	15

$\Gamma = I'$							$\Gamma = I'$						
2μ	2ν	c_1	c_2	c_3	c_4	N	2μ	2ν	c_1	c_2	c_3	c_4	N
5	5	$-i5$		qp^{-2}	qp^3	50	5	$\bar{1}$			$\eta^{-2}qp$	$-\eta^{-1}q$	5
3	5			$\eta^{-1}qp^{-1}$	$-\eta^2 qp^2$	10	3	$\bar{1}$			$-\eta^2 q$	ηqp	5
1	5			$\eta^{-2}q$	$\eta^{-1}qp$	5	1	$\bar{1}$		$i\sqrt{5}\eta$	ηqp	$\eta^{-2}q$	10
$\bar{1}$	5			$\eta^2 qp$	$-\eta q$	5	$\bar{1}$	$\bar{1}$	$-i\sqrt{5}$		q	$-qp$	10
$\bar{3}$	5			ηqp^2	$\eta^{-2}qp^{-1}$	10	$\bar{3}$	$\bar{1}$			$-\eta^{-1}qp$	$-\eta^2 q$	5
$\bar{5}$	5		$-i5$	qp^3	$-qp^{-2}$	50	$\bar{5}$	$\bar{1}$			$-\eta^{-2}q$	$-\eta^{-1}qp$	5
5	3			ηqp^1	$\eta^{-2}qp^2$	10	5	$\bar{3}$			$\eta^{-1}qp^2$	$\eta^2 qp^{-1}$	10
3	3	$-i\sqrt{5}$		qp	q	10	3	$\bar{3}$		$-i\sqrt{5}\eta^{-2}$	$-\eta^{-2}q$	$\eta^{-1}qp$	10
1	3			$-\eta^{-1}qp$	$-\eta^2 q$	5	1	$\bar{3}$			$\eta^2 q$	$-\eta qp$	5
$\bar{1}$	3			$-\eta^{-2}q$	$\eta^{-1}qp$	5	$\bar{1}$	$\bar{3}$			$-\eta qp$	$-\eta^{-2}q$	5
$\bar{3}$	3		$i\sqrt{5}\eta^2$	$-\eta^2 q$	ηqp	10	$\bar{3}$	$\bar{3}$	$-i\sqrt{5}$		$-qp$	$-q$	10
$\bar{5}$	3			$-\eta qp^2$	$-\eta^{-2}qp^{-1}$	10	$\bar{5}$	$\bar{3}$			$\eta^{-1}qp^{-1}$	$-\eta^2 qp^2$	10
5	1			$\eta^2 q$	ηqp	5	5	$\bar{5}$		$i5$	qp^3	$-qp^{-2}$	50
3	1			$-\eta qp$	$-\eta^{-2}q$	5	3	$\bar{5}$			$-\eta^{-1}qp^2$	$-\eta^2 qp^{-1}$	10
1	1	$-i\sqrt{5}$		$-q$	qp	10	1	$\bar{5}$			$\eta^{-2}qp$	$-\eta^{-1}q$	5
$\bar{1}$	1		$-i\sqrt{5}\eta^{-1}$	$\eta^{-1}qp$	$\eta^2 q$	10	$\bar{1}$	$\bar{5}$			$-\eta^2 q$	$-\eta qp$	5
$\bar{3}$	1			$\eta^{-2}q$	$-\eta^{-1}qp$	5	$\bar{3}$	$\bar{5}$			$\eta^{-1}qp^{-1}$	$-\eta^{-2}qp^2$	10
$\bar{5}$	1			$\eta^2 qp$	$-\eta q$	5	$\bar{5}$	$\bar{5}$	$-i5$		$-qp^{-2}$	$-qp^3$	50

$$\psi^{\Gamma_g}_{\mu\nu} = 2^{-1/2}\,(E + P)\,\psi^{\Gamma}_{\mu\nu}, \qquad \psi^{\Gamma_u}_{\mu\nu} = 2^{-1/2}\,(E - P)\,\psi^{\Gamma}_{\mu\nu} \tag{17}$$

4. APPLICATIONS TO THE ANGULAR MOMENTUM STATES

According to the properties (1), one can obtain the irreducible function bases by applying $\psi^{\Gamma}_{\mu\nu}$ to any function. As an important application, one can apply $\psi^{\Gamma}_{\mu\nu}$ to the angular momentum states $|j, \mu\rangle$, where the Condon–Shortley convention is used:

$$R|j, \mu\rangle = \sum_{\nu=-j}^{j} D^{j}_{\nu\mu}(R)|j,\nu\rangle, \qquad R \in SO(3) \text{ or } SU(2) \tag{18}$$

When j is an integer ℓ, the $|\ell, m\rangle$ is nothing but the spherical harmonics $Y^{\ell}_{m}(\theta, \varphi)$. It can be seen from Fig. 1. and (3) that

$$\begin{aligned}
E'|j, \mu\rangle &= (-1)^{2j}|j, \mu\rangle \\
T_0|j, \mu\rangle &= \eta^{\mu}|j, \mu\rangle \\
S_5|j, \mu\rangle &= \sum_{\nu} D^{j}_{\nu\mu}(-2\pi/5,\, 2\theta_4 7\pi/5)|j, \nu\rangle \\
&= \sum_{\nu} e^{-i\mu\pi}\eta^{\mu-\nu}\, d^{j}_{\nu\mu}(2\theta_4)|j, \nu\rangle \\
S_{10}|j, \mu\rangle &= \sum_{\nu} D^{j}_{\nu\mu}(-\pi/5,\, 2\theta_5 6\pi/5)|j, \nu\rangle \\
&= \sum_{\nu} e^{i\nu\pi}\eta^{3\mu+2\nu}\, d^{j}_{\nu\mu}(2\theta_5)|j, \nu\rangle \\
S_{11}|j, \mu\rangle &= \sum_{\nu} D^{j}_{\nu\mu}(0,\, \pi,\, 4\pi/5)|j, \mu\rangle \\
&= (-1)^{j-\mu}\eta^{2\mu}|j, -\mu\rangle
\end{aligned} \tag{19}$$

where $d^{j}(\theta)$ is the D-function in the angular momentum theory [11] and

$$\cos\theta_4 = \sin\theta_5 = q/\sqrt{5}, \qquad \cos\theta_5 = \sin\theta_4 = qp/\sqrt{5} \tag{20}$$

After careful calculation, one can obtain the combinations of the angular momentum states $\psi^{\Gamma}_{\mu\lambda}|j, \rho\rangle$, which belong to the μ row of the irreducible representation Γ of $\mathbf{I}'$:

$$\begin{aligned}
\psi^{\Gamma}_{\mu\lambda}|j, \rho\rangle = \sqrt{10/N}\delta'_{\lambda\rho} \sum_{\nu} \delta'_{\mu\nu}\{&c_1\delta_{\rho\nu} + c_2\delta_{\rho\bar{\nu}}(-1)^{j-\rho}\eta^{2\rho} \\
&+ \sqrt{5}c_3 e^{-i\pi\rho}\eta^{\rho-\nu}\, d^{j}_{\nu\rho}(2\theta_4) + \sqrt{5}c_4 e^{i\pi\nu}\eta^{3\rho+2\nu}\, d^{j}_{\nu\rho}(2\theta_5)\}|j, \nu\rangle
\end{aligned} \tag{21}$$

where N and c_i are also given in Table I. The $\delta'_{\lambda\rho}$ is defined as

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

In the course of obtaining (21), some terms are merged so that the functions need to be normalized again.

Equation (21) is our main formula. For fixed λ and ρ, under the condition $\delta'_{\lambda\rho} = 1$, one can obtain the combinations of the angular momentum states $\psi^{\Gamma}_{\mu\lambda}|j, \rho\rangle$, which belong to the μ row of the irreducible representation Γ of $\mathbf{I}'$. Different choices of λ and ρ may lead to the combinations vanishing, being dependent on each other, or being independent. The number of independent combinations depends upon the number of times that the irreducible representation Γ of $\mathbf{I}'$ appears in the reduced form of the subduced representation of D^j of $SU(2)$. The latter can be completely determined by the character of the representation and is listed in Table 2 of ref. 1. The combinations can be calculated by computer or even by hand. As examples, some combinations are as follows:

$$\psi^{A}_{00}|0, 0\rangle = 2\sqrt{30}|0, 0\rangle \qquad \psi^{T^1}_{\mu 1}|1, 1\rangle = 2\sqrt{10}|1, \mu\rangle$$

$$\psi^{H}_{\mu 2}|2, 2\rangle = 2\sqrt{6}|2, \mu\rangle \qquad \psi^{E'_1}_{\mu(1/2)}|1/2, 1/2\rangle = -i2\sqrt{15}|1/2, \mu\rangle$$

$$\psi^{G'}_{\mu(3/2)}|3/2, 3/2\rangle = i\sqrt{30}|3/2, \mu\rangle, \qquad \psi^{I'}_{\mu(5/2)}|5/2, 5/2\rangle = -i2\sqrt{5}|5/2, \mu\rangle$$

$$\psi^{T_2}_{22}|3, 3\rangle = -4(\sqrt{3/5}|3, 2\rangle + \sqrt{2/5}|3, -3\rangle)$$

$$\psi^{T_2}_{02}|3, 3\rangle = -4|3, 0\rangle$$

$$\psi^{T_2}_{\bar{2}2}|3, 3\rangle = -4(-\sqrt{2/5}|3, 3\rangle + \sqrt{3/5}|3, -2\rangle)$$

$$\psi^{G}_{22}|3, 3\rangle = 3\sqrt{2}(-\sqrt{2/5}|3, 2\rangle + \sqrt{3/5}|3, -3\rangle)$$

$$\psi^{G}_{12}|3, 3\rangle = 3\sqrt{2}|3, 1\rangle$$

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

$$\psi^{G}_{\bar{2}2}|3, 3\rangle = 3\sqrt{2}(\sqrt{3/5}|3, 3\rangle + \sqrt{2/5}|3, -2\rangle)$$

$$\psi^{E'_2}_{3/2\overline{3/2}}|7/2,7/2\rangle = -i3\sqrt{2}(-\sqrt{7/10}|7/2, 3/2\rangle + \sqrt{3/10}|7/2, -7/2\rangle)$$

$$\psi^{E'_2}_{\overline{3/2}\,\overline{3/2}}|7/2, 7/2\rangle = -i3\sqrt{2}(\sqrt{3/10}|7/2, 7/2\rangle + \sqrt{7/10}|7/2, - 3/2\rangle)$$

$$\psi^{I'}_{5/2\overline{3/2}}|7/2, 7/2\rangle = i\sqrt{14}(\sqrt{1/50}|7/2, 5/2\rangle + 7/\sqrt{50}|7/2, - 5/2\rangle)$$

$$\psi^{I'}_{3/2\overline{3/2}}|7/2, 7/2\rangle = i\sqrt{14}(-\sqrt{3/10}|7/2, 3/2\rangle - \sqrt{7/10}|7/2, -7/2\rangle)$$

$$\psi^{I'}_{1/2\overline{3/2}}|7/2, 7/2\rangle = i\sqrt{14}|7/2, 1/2\rangle$$

$$\psi^{I'}_{\overline{1/2}\,\overline{3/2}}|7/2, 7/2\rangle = -i\sqrt{14}|7/2, -1/2\rangle$$

$$\psi^{I'}_{3/23/2}|7/2,\ 7/2\rangle = i\sqrt{14}(-\sqrt{7/10}|7/2,\ 7/2\rangle + \sqrt{3/10}|7/2,\ -3/2\rangle)$$
$$\psi^{I'}_{5/23/2}|7/2,\ 7/2\rangle = i\sqrt{14}(7/\sqrt{50}|7/2,\ 5/2\rangle - \sqrt{1/50}|7/2,\ -5/2\rangle)$$

Other combinations can be obtained by the same method.

5. CONCLUDING REMARKS

If the Hamiltonian of a system has a given symmetry, the symmetry-adapted bases are very useful for calculating the eigenvalues and eigenstates. Generally, the symmetry-adapted bases can be simply obtained from the irreducible bases in the group space of the symmetry group of the system. In this paper, we have explicitly presented the expression for the irreducible bases of **I**$'$ group space. As an important application, the combinations of the angular momentum states into irreducible basis functions belonging to a given row of a given irreducible representation of **I**$'$, which are very crucial for calculating the symmetry-adapted bases, have been presented by a simple and unified formula, (21). Moreover, it is worthwhile to emphasize that the method used in this paper is effective for any double point group.

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