

Algebraic expressions for symmetry-adapted functions of the icosahedral group in spinor space

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Abstract

Algebraic expressions for projection operators and symmetry-adapted functions (SAFs) of the icosahedral group for spinor (double-valued) representations are found by using the double-induced technique and eigenfunction method. The SAFs are functions of the angular momentum j , the quantum numbers λ , ν , μ of the group chain $I \supset D_5 \supset C_5$, and the multiplicity label \bar{m} . By this procedure, SAFs for the group I are provided once for all instead of one j value at a time.

1. Introduction

A significant difficulty with point-group applications is a dependence upon tabulated results. For example, there are many tables of results for the icosahedral group I . Using the $SO_3 \downarrow I$ subduced technique and projection-operator method, the single-valued (s-v) symmetry-adapted functions (SAFs) of I have been calculated by Michel (1992), Cohan (1958) and Elcoro *et al.* (1994), with $l_{\max} = 10, 12, 16$, respectively. Both the s-v and double-valued (d-v) SAFs of I have been obtained by McLellan (1961) for $j = 0, \frac{1}{2}, \dots, 8$. These SAFs are symmetry adapted to the group chain $I \supset C_5$. The $I \supset D_5 \supset C_5$ SAFs for both s-v (vector) and d-v (spinor) representations (reps) have been tabulated for $j = 0-8$ by Butler (1981) using a build-up procedure. Prandl *et al.* (1996) proposed a recursive method for constructing SAFs of I with the totally symmetric SAFs obtained in this way for angular momentum l up to 30.

In Altmann & Herzog (1994), the s-v SAFs of the group chain $I \supset T \supset C_2$ are tabulated out to 12 digits for l up to 15, while the d-v SAFs are given in terms of the so-called *spin harmonics*, which are constructed by coupling the s-v SAFs with the spin wave functions (belonging to the irrep $E_{1/2}$) using Clebsch–Gordan (CG) coefficients in accordance with the CG series, which reads (with the irrep notation of I shown in Table 1)

$$\begin{aligned} F_1 \times E_{1/2} &= E_{1/2} + G_{3/2}, & F_2 \times E_{1/2} &= I_{5/2}, \\ G \times E_{1/2} &= E_{3/2} + I_{5/2}, & H \times E_{1/2} &= G_{3/2} + I_{5/2}. \end{aligned} \quad (1)$$

The spin harmonics are linear combinations of the products of Y_{lm} and spin-wave functions. This representation is rather cumbersome and usually reducible with respect to O_3 . Some low-angular-moment d-v SAFs of I are given as linear combinations of $|jm\rangle$ in Table T74.6a of Altmann & Herzog (1994).

Except for Butler (1981), who introduced a build-up procedure, the conventional scheme for constructing SAFs is the projection-operator method. The construction of SAFs for a high-symmetry group like I using projection is very difficult (Herman, 1997).

So far, we have only considered numerical solutions for determining SAFs of point groups. The shortcomings of numerical results are quite clear. For example, for practical calculations one usually needs various tables, which may not be readily available, and when they are they are frequently subject to printing errors. Another difficulty with tabulated material is that regularities are hard to find. It is highly desirable, therefore, to obtain analytic or algebraic solutions for all point groups, just as we have for the rotation group. Recently, some progress has been made in this direction. For example, algebraic solutions have been reported for all dihedral groups (Chen *et al.*, 1999) and the tetrahedral group (Chen & Fan, 1998a,b,c). What makes an algebraic solution appealing is the fact that the irreducible matrices, projection operators and SAFs are then functions of the quantum numbers (λ, μ) characterizing the group chain [in analogy with (j, m) for $SO_3 \supset SO_2$] and these expressions are valid for both s-v and d-v reps.

In a previous paper (Fan *et al.*, 1999), we used the double-induced technique and eigenfunction method to obtain algebraic solutions for s-v reps of I . Simple algebraic expressions were derived for the SAFs by applying the reduced projection operators $\varphi_{\mu}^{(\lambda)\bar{m}}$ to $Y_{l\bar{m}}$. The reduced projection operator of I contains only 4 terms instead of 60 terms, but plays the same role as the usual projection operator. Therefore, its introduction greatly simplifies the projection-operator method. Indeed, the SAFs are merely functions of the angular momentum l , the quantum numbers λ, μ of the group chain $I \supset C_5$ and the multiplicity label \bar{m} , without involving any irreducible matrix elements. In this way, the s-v SAFs problem of I has been solved once for all

Table 1. The subduction rule for $I \downarrow D_5 \downarrow C_5$ and eigenvalues (λ, ρ) of (C, C_{5z})

I	$E_{1/2}$	$E_{3/2}$	$G_{3/2}$	$I_{5/2}$
	$12c_{1/2}$	$12c_{3/2}$	3	-2
D_5	$E_{1/2}$	$E_{3/2}$	$E_{1/2}$ $E_{3/2}$	$E_{1/2}$ $E_{3/2}$ $[+\frac{3}{5}]$ $[-\frac{2}{5}]$
μ	$(\frac{1}{2}, -\frac{1}{2})$	$(\frac{3}{5}, -\frac{2}{5})$	$(\frac{1}{2}, -\frac{1}{2})$ $(\frac{3}{5}, -\frac{2}{5})$	$(\frac{1}{2}, -\frac{1}{2})$ $(\frac{3}{5}, -\frac{2}{5})$ $\frac{1}{2}$ $\frac{5}{2}$

The four irreps of I are labelled as $E_{1/2}, E_{7/2}, F_{3/2}, I_{5/2}$ in Altmann & Herzog (1994) and as $\frac{1}{2}, \frac{7}{2}, \frac{3}{2}, \frac{5}{2}$ in Butler (1981). The eigenvalue ρ is related to the irrep label μ of C_5 by $\rho = \exp(-2\mu\pi i/5)$.

instead of one angular momentum l at a time. The purpose of this study is to extend the treatment of the s-v reps of I to its d-v reps, so we can have a complete algebraic solution for the icosahedral group.

2. The representation group

We restrict ourselves to the proper point groups, since an extension to the improper point groups is straightforward. In dealing with spinor reps, it is useful to begin with a brief introduction of the double-point-group concept. Consider a point group \hat{G}

$$\hat{G} = \{\hat{R}_i : i = 1, 2, \dots, |G|\}, \quad \hat{R}_i = R_{\mathbf{n}_i}(\omega_i), \quad (2)$$

where $R_{\mathbf{n}_i}(\omega_i)$ denotes a rotation about the axis \mathbf{n}_i through angle ω_i . The corresponding double point group is

$$\hat{G}^\dagger = \{\hat{R}_i, \tilde{\hat{R}}_i : i = 1, 2, \dots, |G|\}, \quad \tilde{\hat{R}}_i = R_{\mathbf{n}_i}(\omega_i + 2\pi). \quad (3)$$

We use R_i, \tilde{R}_i to denote the corresponding operators, or matrices, of

$$\hat{R}_i, \tilde{\hat{R}}_i$$

in a generic representation space. Rotations through an angle φ and $\varphi + 2\pi$ are identical in a vector representation space but differ in sign in a spinor representation space. Therefore, in spinor space,

$$\tilde{R}_i = -R_i. \quad (4)$$

A convenient way of dealing with the d-v reps of a point or space group is by means of the so-called *representation group (rep group)* first introduced by Chen *et al.* (1985).

Definition 1. The representation of a group \hat{G} in a representation space r forms a group, called the *representation group (rep group)* \mathcal{G}_r .

Remark 1. The representation r may be reducible or irreducible and may be faithful or unfaithful. In this study, we are interested in faithful and reducible rep groups only; unfaithful rep groups find their application in Chen & Fan (1998b, p. 5505).

The elements R_a, R_b, \dots of \mathcal{G}_r are matrices or operators and if $R_a = \varepsilon R_b$, where ε is a complex number

with $|\varepsilon| = 1$, R_a and R_b are said to be linearly dependent, otherwise they are linearly independent.

Definition 2. The number of linearly independent elements of \mathcal{G}_r is called the order of the rep group, denoted by $|\mathcal{G}_r|$.

Remark 2. A fundamental difference between a rep group and an ordinary group (*i.e.* a group in the usual sense) is that the elements of the former may be *linearly dependent* while those of the latter are always linearly independent. When all elements of a rep group are linearly independent, it reduces to the ordinary group. In this sense, the ordinary group can be regarded as a special case of the rep group.

Remark 3. A rep group differs from a matrix group in the sense that for the latter all elements (matrices) are regarded as linearly independent. For example, the quaternion group Q ,

$$Q = \{\pm e, \pm i\sigma_x, \pm i\sigma_y, \pm i\sigma_z\},$$

which is isomorphic to the double group D_2^\dagger ($C_{2k} \sim -i\sigma_k, \tilde{C}_{2k} \sim i\sigma_k, k = x, y, z$), is of order 8, since all elements are regarded as linearly independent. The set of these eight matrices could also be regarded as a rep group \mathcal{Q} with four linearly independent elements.

Remark 4. The rep group used here is to be distinguished from the representation group defined by Döring (1959) and Birman (1974), which is a group in the usual sense.

Remark 5. Owing to the linear dependence of its elements, the class operators (a class operator is a sum of all elements belonging to the same class) of a rep group are also linearly dependent: some may be null operators and some may only differ in signs.

It is important to note that for the rep group we have the generalized Burnside theorem (Chen *et al.*, 1985, p. 230):

Theorem 1. A rep group \mathcal{G}_r has N inequivalent irreps, N being the number of linearly independent class operators of \mathcal{G}_r ; the number of times each irrep occurs in the representation space r is equal to its dimensions and the sum of the squares of the dimensions of all irreps is equal to the order $|\mathcal{G}_r|$,

$$\sum_{i=1}^N |\lambda_i|^2 = |\mathcal{G}_r|. \quad (5)$$

Example 1. The rep groups \mathcal{G}_r of the inversion group $\hat{G} = (\hat{e}, \hat{I})$ in the representation spaces $r = g, u$ associated with $I = 1, -1$ are $\mathcal{G}_g = (e, e)$ and $\mathcal{G}_u = (e, -e)$, respectively. The former is unfaithful while the latter is faithful, and both have only one linearly independent element. According to Theorem 1, both only have one one-dimensional irrep, and they are just the rep groups themselves.

Example 2. The quaternion group Q has five classes with class operators

$$\begin{aligned} C_1 &= e, & C_2 &= -e, & C_3 &= (i\sigma_x) + (-i\sigma_x), \\ C_4 &= (i\sigma_y) + (-i\sigma_y), & C_5 &= (i\sigma_z) + (-i\sigma_z). \end{aligned}$$

The group $Q \sim D_2^\dagger$ has five irreps, four one-dimensional and one two-dimensional. On the other hand, the rep group \mathcal{Q} has only one linearly independent class operator, $C_1 = -C_2 = e, C_3 = C_4 = C_5 = 0$. According to Theorem 1, the rep group \mathcal{Q} has a single irrep, which according to (5) is two-dimensional and is just the representation group \mathcal{Q} itself. \mathcal{Q} is the spinor irrep of the dihedral group D_2 .

In the above examples, the representations on which the rep groups are defined are irreducible. What we are interested in are the cases where the representations are reducible, and we now turn to the double group G^\dagger .

Example 3. The representation of G^\dagger in a generic spinor space forms a rep group \mathcal{G} of order $|G|$,

$$\mathcal{G} = \{R_i, -R_i : i = 1, \dots, |G|\}. \quad (6)$$

Definition 3. The $|G|$ -dimensional space $\{R_i : i = 1, \dots, |G|\}$ is called the group space of \mathcal{G} , which carries a representation space of \mathcal{G} called the *regular representation* of \mathcal{G} .

The multiplication table of \mathcal{G} is obtained from that of G^\dagger by replacing (\hat{R}_i, \bar{R}_i) with $(R_i, -R_i)$. The regular representation of \mathcal{G} is in general reducible and our central task is to decompose it into irreps.

Several methods are available for finding d-v irreps of a group G ; four of interest to us follow: (i) the double-group method (Bradley & Cracknell, 1972); (ii) the subduction method (McLellan, 1961); (iii) the representation group method where the problem of seeking the d-v irreps of G is equivalent to that of seeking the irreps of the rep group \mathcal{G} of order $|G|$ (Chen *et al.*, 1985); and (iv) the projective representation method (Altmann, 1986). Obviously, the third approach is much simpler than the first one, since the order \mathcal{G} is one half of that of the group G^\dagger .

The treatment of the rep group \mathcal{I} is exactly the same as for the s-v reps of the group I presented in Fan *et al.*

(1999) but with a few modifications noted below. In the following, we deal only with the rep group and for simplicity we shall just say the ‘group’ instead of the ‘rep group’ and use the notation I, D_5, C_5 instead of $\mathcal{I}, \mathcal{D}_5, \mathcal{C}_5$ for the respective rep groups.

3. The $I \supset D_5 \supset C_5$ projection operators

The rotation axes and the Euler angles of the 60 elements of the group I are shown in Fig. 1 and Tables 1 and 2 of Fan *et al.* (1999). With the Euler angles and the rotation matrices $D^{1/2}(\alpha, \beta, \gamma)$ (Rose, 1957), the group table of the double point group I^\dagger can be constructed and is available upon request from JQC.

We first review the s-v case given in Fan *et al.* (1999). A key for constructing SAFs is to find the projection operator. The normalized generalized projection operator for the group chain $I \supset C_5$ is defined as

$$\mathcal{P}_\mu^{(\lambda)\bar{\mu}} = (h_\lambda/60)^{1/2} \sum_{a=1}^{60} D_{\mu\bar{\mu}}^{(\lambda)}(R_a)^* R_a, \quad (7)$$

where h_λ is the dimension of the irrep λ , $D^{(\lambda)}(R_a)$ is the irreducible matrix of the element R_a and μ is the quantum number of the cyclic group C_5 generated from $C_{5z} = C_{5,6}$. For brevity, the generalized projection operator is referred to as the projection operator.

Consider the double-coset decomposition of I with respect to the subgroup C_5 ,

$$I = \sum_{i=1}^4 C_5 \hat{\beta}_i C_5 = C_5 (\hat{\beta}_1 + \hat{\beta}_2) + C_5 (\hat{\beta}_3 + \hat{\beta}_4) C_5, \quad (8a)$$

with the coset representatives chosen as

$$\hat{\beta}_1 = e, \quad \hat{\beta}_2 = C_{2,8}, \quad \hat{\beta}_3 = C_{2,13}, \quad \hat{\beta}_4 = C_{2,5}. \quad (8b)$$

The projection operator (7) can be factorized into a product of the projection operators $P^\mu, P^{\bar{\mu}}$ of C_5 and the *reduced projection operator* $\wp_\mu^{(\lambda)\bar{\mu}}$,

$$\mathcal{P}_\mu^{(\lambda)\bar{\mu}} = (h_\lambda/60)^{1/2} P^\mu \wp_\mu^{(\lambda)\bar{\mu}} P^{\bar{\mu}}, \quad (9a)$$

$$\wp_\mu^{(\lambda)\bar{\mu}} = \sum_{i=1}^4 M_i^{-1} d_{\mu\bar{\mu}}^{(\lambda)}(\hat{\beta}_i)^* \hat{\beta}_i, \quad (9b)$$

where P^μ is the projection operator of C_5 and M_i is the number of the times an element appears in the double coset $C_5 \hat{\beta}_i C_5$,

$$M_i = \begin{cases} 5, & i = 1, 2 \\ 1, & i = 3, 4. \end{cases} \quad (10)$$

The $I \supset C_5$ projection operator $\mathcal{P}_\mu^{(\lambda)\bar{\mu}}$ fulfils the following set of eigenvalue equations:

$$(C, C_{5z}, \bar{C}_{5z}) \mathcal{P}_\mu^{(\lambda)\bar{\mu}} = (\lambda, \rho_\mu, \rho_{\bar{\mu}}) \mathcal{P}_\mu^{(\lambda)\bar{\mu}}, \quad (11)$$

where C and C_{5z} are the CSCO (complete set of commuting operators) (Chen, 1989) of I and C_5 , the quantum numbers λ, μ are labels of the irreps of I and

C_5 , and \bar{C}_{5z} is the intrinsic operator, which is the operator C_{5z} acting from the right, $\bar{C}_{5z}\mathcal{P}_\mu^{(\lambda)\bar{\nu}\bar{\mu}} = \mathcal{P}_\mu^{(\lambda)\bar{\nu}\bar{\mu}}C_{5z}$.

The modifications necessary for extending the method of Fan *et al.* (1999) for the s-v case to the d-v case are:

Modification 1. Possible eigenvalues of the CSCO,

$$C = \sum_{j=1}^6 [C_{5,j} + C_{5,j}^-], \quad (12)$$

of I in a generic spinor space are

$$12c_{1/2}[= 3 + 3(5)^{1/2}], \quad 12c_{3/2}[= 3 - 3(5)^{1/2}], \quad 3, \quad -2, \quad (13)$$

with $c_\mu = \cos(2\pi\mu/5)$, which correspond to the four d-v irreps, $(E_{1/2}, E_{3/2}, G_{3/2}, I_{5/2})$ in the modified Mulliken notation, as shown in Table 1. As will be seen later, this notation is very convenient for obtaining algebraic expressions of the projection operators. The eigenvalues λ^Γ of C for the irrep Γ in (13) can be found by solving the eigenvalue equation of C shown in (20b) or by the known character χ_i^Γ for the class i , $\{C_{5,j}, C_{5,j}^-; j = 1, \dots, 6\}$, through the relation

$$\lambda^\Gamma = g_i \chi_i^\Gamma / h_\Gamma,$$

where h_Γ is the dimension of the irrep Γ and $g_i = 12$ is the number of elements in the class $\{C_{5,j}, C_{5,j}^-; j = 1, \dots, 6\}$.

Modification 2. The operator

$$C_{5,6} = C_{5z} = \exp(-2\pi J_z i / 5) \quad (14)$$

remains the CSCO of C_5 but C_{5z}^5 is no longer equal to the identity operator e . Instead, we have $C_{5z}^5 = -e$. In a spinor space, the operator C_{5z} has five distinct eigenvalues:

$$\rho \equiv \rho_\mu = \exp(-2\pi\mu i / 5), \quad \mu = \pm\frac{1}{2}, \pm\frac{3}{2}, \frac{5}{2}. \quad (15)$$

Note that

$$(\rho)^{5+k} = -\rho^k, \quad C_{5z}^{5+k} = -C_{5z}^k,$$

$$\rho_{1/2} = -\rho_{-2}, \quad \rho_{3/2} = -\rho_{-1}, \quad \rho_{5/2} = -\rho_0 = -1.$$

The unnormalized projection operator P^μ in (9a) of the cyclic group C_5 is defined as

$$P^\rho \equiv P^\mu = \frac{1}{2} \sum_{k=0}^9 (\rho^*)^k (C_{5z})^k \\ = e + \rho^* C_{5z} + \rho^{*2} C_{5z}^2 + \rho^2 C_{5z}^{-2} + \rho C_{5z}^-. \quad (16)$$

Modification 3. For the d-v case, the group chain $I \supset D_5 \supset C_5$ is canonical while $I \supset C_5$ is not. The $I \supset D_5 \supset C_5$ projection operator is denoted by $\mathcal{P}_{\nu\mu}^{(\lambda)\bar{\nu}\bar{\mu}}$ and obeys the eigenvalue equations

$$(C, C_{D_5}, C_{5z}, \bar{C}_{D_5}, \bar{C}_{5z}) \mathcal{P}_{\nu\mu}^{(\lambda)\bar{\nu}\bar{\mu}} = (\lambda, \nu, \rho_\mu, \bar{\nu}, \rho_{\bar{\mu}}) \mathcal{P}_{\nu\mu}^{(\lambda)\bar{\nu}\bar{\mu}}, \quad (17)$$

where C_{D_5} and \bar{C}_{D_5} are the CSCO of D_5 and the intrinsic group \bar{D}_5 . From the subduction rule (Butler, 1981) shown in Table 1, it is known that the subgroup D_5 is redundant for all cases except $\mu = \frac{5}{2}$. Therefore, for $\mu \neq \frac{5}{2}$, the eigenvalue equations for C_{D_5} and C_{D_5} in (17) are redundant. On the other hand, the irrep $\mu = \frac{5}{2}$ of C_5 occurs twice in the irrep $I_{5/2}$, which is distinguished by the irreps $[+\frac{5}{2}]$, $[-\frac{5}{2}]$ of D_5 in Butler's (1981) notation (the square brackets are added here to distinguish them from the quantum number $\mu = \pm\frac{5}{2}$) or Γ_7 , Γ_8 in the Koster *et al.* (1963) notation. Since the irreps $[\pm\frac{5}{2}]$ of D_5 are one-dimensional, the diagonalization of (C_{D_5}, \bar{C}_{D_5}) can be replaced by a much simpler procedure, that is, by the diagonalization of a single twofold rotation of D_5 and its intrinsic counterpart, for example, $(C_{2,8}, \bar{C}_{2,8})$.

A discussion of the labelling is in order for the $I \supset D_5 \supset C_5$ basis. From Table 1, it can be seen that for $\mu \neq \frac{5}{2}$ the ν label of D_5 is redundant,

$$(\lambda, E_{|\mu|}, \mu) \rightarrow (\lambda, \mu), \quad \mu = \pm\frac{1}{2}, \pm\frac{3}{2}.$$

When $\nu = [\pm\frac{5}{2}]$, the quantum number $\mu = \frac{5}{2}$ is redundant,

$$(\lambda, [\pm\frac{5}{2}], \frac{5}{2}) \rightarrow (\lambda, [\pm\frac{5}{2}]).$$

Therefore, the $I \supset D_5 \supset C_5$ irreducible basis can still be labelled by two quantum numbers (λ, μ) but with the above extended meaning for $\mu = [\pm\frac{5}{2}]$,

$$(\lambda, \mu), \quad \mu = \pm\frac{1}{2}, \pm\frac{3}{2}, [\pm\frac{5}{2}].$$

As for the s-v case, the following orthonormal vectors,

$$\begin{aligned} \phi_{\mu\bar{\mu}}^1 &= \delta_{\mu\bar{\mu}} \phi_\mu^1, & \phi_{\mu\bar{\mu}}^2 &= \delta_{\mu-\bar{\mu}} \phi_\mu^2, \\ \phi_{\mu\bar{\mu}}^3 &= \frac{1}{5} P^\mu C_{2,13} P^{\bar{\mu}}, & \phi_{\mu\bar{\mu}}^4 &= \frac{1}{5} P^\mu C_{2,5} P^{\bar{\mu}}, \end{aligned} \quad (18a)$$

form the double-induced representation $(\mu, \bar{\mu})$, where

$$\phi_\mu^1 = (1/5^{1/2}) P^\mu, \quad \phi_\mu^2 = (1/5^{1/2}) P^\mu C_{2,8}. \quad (18b)$$

There are altogether $5 + 5 + 25 + 25 = 60$ linearly independent basis vectors in (18a) and (18b), which is just the order of the rep group I .

The representation matrix M of the CSCO of the group I in the double-induced representation $(\mu, \bar{\mu})$ is

$$M_{ij}(\mu, \bar{\mu}) = \langle \phi_{\mu\bar{\mu}}^i | C | \phi_{\mu\bar{\mu}}^j \rangle. \quad (19)$$

The projection operators can be expressed as

$$\mathcal{P}_\mu^{(\lambda)\bar{\mu}} = \sum_{i=1}^4 u_{i,\mu\bar{\mu}}^{(\lambda)} \phi_{\mu\bar{\mu}}^i, \quad (20a)$$

and the coefficients $u_i \equiv u_{i,\mu\bar{\mu}}^{(\lambda)}$ are determined from the matrix equation

$$M(\mu, \bar{\mu}) \mathbf{u}_{\mu\bar{\mu}}^{(\lambda)} = \lambda \mathbf{u}_{\mu\bar{\mu}}^{(\lambda)}, \quad (20b)$$

Table 2. The value of s_μ , c_μ and t_μ

$c_{1/2} = -c_2$ $(1 + 5^{1/2})/4$	$c_{3/2} = -c_1$ $(1 - 5^{1/2})/4$	$s_1 = s_{3/2}$ $[10 + 2(5)^{1/2}]^{1/2}/4$	$s_2 = s_{1/2}$ $[10 - 2(5)^{1/2}]^{1/2}/4$
$t_1 = -t_{3/2}$ $[5 + 2(5)^{1/2}]^{1/2}$	$t_2 = -t_{1/2}$ $[-5 - 2(5)^{1/2}]^{1/2}$	$s_2 c_1^2$ $[50 - 22(5)^{1/2}]^{1/2}/16$	$s_1 c_2^2$ $[50 + 22(5)^{1/2}]^{1/2}/16$

where $\mathbf{u} = \{u_1, \dots, u_4\}_{\text{column}}$ are orthonormalized column vectors.

Using the group table of I^\dagger and techniques similar to those used in Chen & Fan (1998a), we can determine the action of C in the double-induced representation, which can be simplified as

$$\begin{aligned}
 C\phi_\mu^1 &= 2c_\mu\phi_\mu^1 + 2(5)^{1/2}is_{2\mu}\phi_{\mu\mu}^4, \\
 C\phi_\mu^2 &= 2c_\mu\phi_\mu^2 - 2(5)^{1/2}is_{2\mu}\phi_{\mu-\mu}^3, \\
 C\phi_{\mu\bar{\mu}}^3 &= 2(5)^{1/2}is_{2\mu}\delta_{\mu-\bar{\mu}}\phi_\mu^2 + 2(c_\mu + c_{\bar{\mu}} + c_{\mu+\bar{\mu}})\phi_{\mu\bar{\mu}}^3 \\
 &\quad - 2(c_{2\mu+2\bar{\mu}} + c_{3\mu+2\bar{\mu}})\phi_{\mu\bar{\mu}}^4, \\
 C\phi_{\mu\bar{\mu}}^4 &= -2(5)^{1/2}is_{2\mu}\delta_{\mu\bar{\mu}}\phi_\mu^1 - 2(c_{2\mu+2\bar{\mu}} + c_{3\mu+2\bar{\mu}})\phi_{\mu\bar{\mu}}^3 \\
 &\quad + 2(c_\mu + c_{\bar{\mu}} + c_{\mu-\bar{\mu}})\phi_{\mu\bar{\mu}}^4.
 \end{aligned} \tag{21}$$

From (21), we get the matrix M ,

$$M = 2 \begin{bmatrix} c_\mu \delta_{\mu\bar{\mu}} & 0 & 0 & -i5^{1/2}s_{2\mu}\delta_{\mu\bar{\mu}} \\ 0 & c_\mu \delta_{\mu-\bar{\mu}} & i5^{1/2}s_{2\mu}\delta_{\mu-\bar{\mu}} & 0 \\ 0 & -i5^{1/2}s_{2\mu}\delta_{\mu-\bar{\mu}} & c_\mu + c_{\bar{\mu}} + c_{\mu+\bar{\mu}} & -c_{2\mu+2\bar{\mu}} - c_{3\mu+2\bar{\mu}} \\ i5^{1/2}s_{2\mu}\delta_{\mu\bar{\mu}} & 0 & -c_{2\mu+2\bar{\mu}} - c_{3\mu+2\bar{\mu}} & c_{\bar{\mu}} + c_\mu + c_{\mu-\bar{\mu}} \end{bmatrix}. \tag{22}$$

Here and below, we use the following three symbols for commonly occurring quantities:

$$\begin{aligned}
 c_\mu &= \cos(2\mu\pi/5), & s_\mu &= \sin(2\mu\pi/5), \\
 t_\mu &= \tan(2\mu\pi/5).
 \end{aligned} \tag{23}$$

The table of numerical values for these quantities is shown in Table 2. There exist many useful relations between these quantities:

$$\begin{aligned}
 c_{-\mu} &= c_\mu, & s_{-\mu} &= -s_\mu, \\
 c_1 &= c_4 = -c_{3/2}, & c_2 &= c_3 = -c_{1/2}, \\
 s_1 &= -s_4 = s_{3/2}, & s_2 &= -s_3 = s_{1/2}, \\
 t_1 &= -t_4 = -t_{3/2}, & t_2 &= -t_3 = -t_{1/2}.
 \end{aligned} \tag{24}$$

The eigenvectors of the matrix M will be obtained separately in four cases:

Case (i). $\mu = \bar{\mu} = \pm\frac{1}{2}, \pm\frac{3}{2}$ ($\rho = \bar{\rho} \neq \text{real}$).

In this case, the matrix M is three-dimensional. In the basis $\phi_\mu^1, \phi_{\mu\mu}^3$ and $\phi_{\mu-\mu}^4$,

$$M = 2 \begin{pmatrix} c_\mu & 0 & -i5^{1/2}s_{2\mu} \\ 0 & 2c_\mu + c_{2\mu} & c_\mu + 1 \\ i5^{1/2}s_{2\mu} & c_\mu + 1 & 2c_\mu + 1 \end{pmatrix} \tag{25}$$

with eigenvectors

$$\begin{aligned}
 \mathcal{P}_\mu^{(\lambda)\mu} &= N_\lambda \left[\phi_\mu^1 + \frac{i(\lambda - 2c_\mu)(c_\mu + 1)}{5^{1/2}s_{2\mu}(\lambda - 4c_\mu - 2c_{2\mu})} \phi_{\mu\mu}^3 \right. \\
 &\quad \left. + i \frac{\lambda - 2c_\mu}{2(5)^{1/2}s_{2\mu}} \phi_{\mu-\mu}^4 \right]
 \end{aligned} \tag{26}$$

and eigenvalues $\lambda = 3, -2, 12c_\mu$.

Equation (26) gives the algebraic expression of the projection operators as a function of λ . This expression is very elegant if the quantum number λ is used as an irrep label. Unfortunately, most are not familiar with this new labelling scheme and therefore it is more convenient to change back to the Mulliken notation. From (26) and Table 1, we obtain the projection operators in a more explicit but less compact form:

$$\begin{cases} \mathcal{P}_\mu^{(G_{3/2})\mu} = (1/3^{1/2})[\phi_\mu^1 - (i/5^{1/2})t_{2\mu}\phi_{\mu\mu}^3 \\ \quad + (i/5^{1/2})t_\mu\phi_{\mu\mu}^4] \\ \mathcal{P}_\mu^{(I_{5/2})\mu} = (1/2^{1/2})[\phi_\mu^1 + (i/5^{1/2})2s_\mu\phi_{\mu\mu}^3 \\ \quad - (i/5^{1/2})2s_{2\mu}\phi_{\mu\mu}^4], & \mu = \pm\frac{1}{2}, \pm\frac{3}{2} \\ \mathcal{P}_\mu^{(E_{|\mu|})\mu} = (1/6^{1/2})[\phi_\mu^1 + (i/2)5^{1/2}s_{2\mu}^{-1}\phi_{\mu\mu}^3 \\ \quad + (i/2)5^{1/2}s_\mu^{-1}\phi_{\mu-\mu}^4], \end{cases} \tag{27}$$

where $t_\mu = s_\mu/c_\mu$.

Case (ii). $\mu = -\bar{\mu} = \pm\frac{1}{2}, \pm\frac{3}{2}$ ($\rho = \bar{\rho}^* \neq \text{real}$).

The matrix M is again three-dimensional. In the basis $\phi_\mu^2, \phi_{\mu-\mu}^3$ and $\phi_{\mu-\mu}^4$,

$$M = 2 \begin{pmatrix} c_\mu & i5^{1/2}s_{2\mu} & 0 \\ -i5^{1/2}s_{2\mu} & 2c_\mu + 1 & -c_\mu - 1 \\ 0 & -c_\mu - 1 & 2c_\mu + c_{2\mu} \end{pmatrix}. \tag{28}$$

The eigenvalues are the same as for case (i), while the eigenvectors are given by

$$\begin{aligned}
 \mathcal{P}_\mu^{(\lambda)-\mu} &= N_\lambda \left[\phi_\mu^2 - i \frac{\lambda - 2c_\mu}{2(5)^{1/2}s_{2\mu}} \phi_{\mu-\mu}^3 \right. \\
 &\quad \left. + \frac{i(\lambda - 2c_\mu)(c_\mu + 1)}{5^{1/2}s_{2\mu}(\lambda - 4c_\mu - 2c_{2\mu})} \phi_{\mu-\mu}^4 \right].
 \end{aligned} \tag{29}$$

This gives

$$\begin{cases} \mathcal{P}_\mu^{(G_{3/2})-\mu} = (1/3^{1/2})[\phi_\mu^2 - (i/5^{1/2})t_\mu\phi_{\mu-\mu}^3 \\ \quad - (i/5^{1/2})t_{2\mu}\phi_{\mu-\mu}^4] \\ \mathcal{P}_\mu^{(I_{5/2})-\mu} = (1/2^{1/2})[\phi_\mu^2 + (i/5^{1/2})2s_{2\mu}\phi_{\mu-\mu}^3 \\ \quad + (i/5^{1/2})2s_\mu\phi_{\mu-\mu}^4], \quad \mu = \pm\frac{1}{2}, \pm\frac{3}{2} \\ \mathcal{P}_\mu^{(E_{\mu})-\mu} = (1/6^{1/2})[\phi_\mu^2 - (i/2)5^{1/2}s_\mu^{-1}\phi_{\mu-\mu}^3 \\ \quad + (i/2)5^{1/2}s_{2\mu}^{-1}\phi_{\mu-\mu}^4]. \end{cases} \quad (30)$$

Case (iii). $(\mu : \bar{\mu}) = (\pm\frac{1}{2}, \pm\frac{3}{2})$.

We use the symbol $(\mu : \bar{\mu})$ to denote $(\mu, \bar{\mu})$ or $(\bar{\mu}, \mu)$. Now $\phi^1 = \phi^2 \equiv 0$ and the double-induced representation becomes two-dimensional. In the basis $(\phi_{\mu\bar{\mu}}^3, \phi_{\mu\bar{\mu}}^4)$, the matrix M simplifies to

$$M = 2 \begin{pmatrix} c_{\bar{\mu}} + c_\mu + c_{\mu+\bar{\mu}} & -(c_{2\mu+2\bar{\mu}} + c_{3\mu+2\bar{\mu}}) \\ -(c_{2\mu+2\bar{\mu}} + c_{3\mu+2\bar{\mu}}) & c_\mu + c_{\bar{\mu}} + c_{\mu-\bar{\mu}} \end{pmatrix}. \quad (31)$$

This matrix has the nondegenerate eigenvalues 3 and -2 with the eigenvectors

$$\mathcal{P}_\mu^{(\lambda)\bar{\mu}} = N_\lambda \left[\phi_{\mu\bar{\mu}}^3 - \frac{\lambda - 2c_\mu - 2c_{\bar{\mu}} - 2c_{\mu+\bar{\mu}}}{2c_{2\mu+2\bar{\mu}} + 2c_{3\mu+2\bar{\mu}}} \phi_{\mu\bar{\mu}}^4 \right], \quad \lambda = 3, -2. \quad (32)$$

That is,

$$\begin{cases} \mathcal{P}_\mu^{(I_{5/2})\bar{\mu}} = (2/5^{1/2})[s_{2(\mu+\bar{\mu})}\phi_{\mu\bar{\mu}}^3 - s_{\mu+\bar{\mu}}\phi_{\mu\bar{\mu}}^4], \\ \mathcal{P}_\mu^{(G_{3/2})\bar{\mu}} = (2/5^{1/2})[s_{2(\mu-\bar{\mu})}\phi_{\mu\bar{\mu}}^3 - s_{\mu-\bar{\mu}}\phi_{\mu\bar{\mu}}^4], \end{cases} \quad (\mu : \bar{\mu}) = (\pm\frac{1}{2}, \pm\frac{3}{2}). \quad (33)$$

Case (iv). μ or/and $\bar{\mu}$ are equal to $\frac{5}{2}$.

When $\mu = \bar{\mu} = \frac{5}{2}$, the matrix in (22) reduces to $-2 \times \mathbf{I}$, where \mathbf{I} is a 4×4 unit matrix, and it has a fourfold root $\lambda = -2$, corresponding to the six-dimensional irrep $I_{5/2}$. For $\lambda = -2$, we have four linearly independent eigenvectors,

$$\phi_{\frac{5}{2}}^1, \quad \phi_{\frac{5}{2}}^2, \quad \phi_{\frac{5}{2}\frac{5}{2}}^3, \quad \phi_{\frac{5}{2}\frac{5}{2}}^4. \quad (34)$$

When $(\mu : \bar{\mu}) = (\frac{5}{2}, \pm\frac{1}{2}), (\frac{5}{2}, \pm\frac{3}{2})$, the matrix in (31) becomes $-2 \times \mathbf{I}$, where \mathbf{I} is a 2×2 unit matrix, and its eigenvalue $\lambda = -2$ has double degeneracy. The two linearly independent eigenvectors are

$$\phi_{\mu\bar{\mu}}^3, \quad \phi_{\mu\bar{\mu}}^4, \quad (\mu : \bar{\mu}) = (\frac{5}{2}, \pm\frac{3}{2}), (\frac{5}{2}, \pm\frac{1}{2}). \quad (35)$$

From (34) and (35), we know that for either μ or $\bar{\mu}$ equal to $\frac{5}{2}$ the eigenvectors of $(C, C_{5/2}, \bar{C}_{5/2})$ still have degeneracy and we need to use the operators $C_{2,8}$ and $\bar{C}_{2,8}$ to lift the degeneracy by diagonalizing $C_{2,8}$ and $\bar{C}_{2,8}$ in the space $\{\phi_\mu^1, \phi_\mu^2, \phi_{\mu\bar{\mu}}^3, \phi_{\mu\bar{\mu}}^4\}$ with μ or/and $\bar{\mu} = \frac{5}{2}$.

Using the group table of I^\dagger and (18a), we obtain

$$C_{2,8}\phi_{\frac{5}{2}}^1 = \phi_{\frac{5}{2}}^2, \quad C_{2,8}\phi_{\frac{5}{2}\bar{\mu}}^3 = -\phi_{\frac{5}{2}\bar{\mu}}^4, \quad \bar{\mu} = \pm\frac{1}{2}, \pm\frac{3}{2}, \frac{5}{2} \quad (36a)$$

$$\bar{C}_{2,8}\phi_{\frac{5}{2}}^1 = \phi_{\frac{5}{2}}^2, \quad \bar{C}_{2,8}\phi_{\mu\frac{5}{2}}^3 = \phi_{\mu\frac{5}{2}}^4, \quad \mu = \pm\frac{1}{2}, \pm\frac{3}{2}, \frac{5}{2}. \quad (36b)$$

Note that from $C_{2,8}|x\rangle = |y\rangle$, $\bar{C}_{2,8}|x'\rangle = |y'\rangle$, we have $C_{2,8}|y\rangle = -|x\rangle$, $\bar{C}_{2,8}|y'\rangle = -|x'\rangle$, due to $C_{2,8}^2 = -e$. And using (36), we obtain the common eigenvectors of $C_{2,8}$ and $\bar{C}_{2,8}$ in the spaces (34) and (35):

$$\begin{cases} \mathcal{P}_{[\pm\frac{5}{2}]}^{(I_{5/2})[\pm\frac{5}{2}]} = (1/2^{1/2})(\phi_{\pm\frac{5}{2}}^1 \pm i\phi_{\pm\frac{5}{2}}^2), \\ \mathcal{P}_{[\pm\frac{5}{2}]}^{(I_{5/2})[\mp\frac{5}{2}]} = (1/2^{1/2})(\phi_{\pm\frac{5}{2}}^3 \mp i\phi_{\pm\frac{5}{2}}^4), \\ \mathcal{P}_\mu^{(I_{5/2})[\pm\frac{5}{2}]} = (1/2^{1/2})(\phi_{\mu\frac{5}{2}}^3 \pm i\phi_{\mu\frac{5}{2}}^4), \quad \mu = \pm\frac{1}{2}, \pm\frac{3}{2}, \\ \mathcal{P}_{[\pm\frac{5}{2}]}^{(I_{5/2})\bar{\mu}} = (1/2^{1/2})(\phi_{\pm\frac{5}{2}\bar{\mu}}^3 \mp i\phi_{\pm\frac{5}{2}\bar{\mu}}^4), \quad \bar{\mu} = \pm\frac{1}{2}, \pm\frac{3}{2}, \end{cases} \quad (37)$$

where we used the fact that the eigenvalues $\nu = -i$ and i of $C_{2,8}$ correspond to the one-dimensional irreps $[\pm\frac{5}{2}]$ and $[-\frac{5}{2}]$ of D_5 , respectively.

4. The $I \supset D_5 \supset C_5$ reduced projection operators

Substituting (18a,b) into (27), (30), (33) and (37) and choosing appropriate phase factors as described in Fan *et al.* (1999), we get the projection operators $\mathcal{P}_\mu^{(\lambda)\bar{\mu}}$ in terms of $P^\mu \hat{\beta}_i P^{\bar{\mu}}$. According to (9), by deleting the factor $(h_\lambda/60)^{1/2} P^\mu P^{\bar{\mu}}$, we obtain the following reduced projection operators:

$$\begin{cases} \wp_\mu^{(E_\sigma)\mu} = \frac{1}{5}\hat{e} + (i/2)[s_{2\mu}^{-1}\hat{\beta}_3 + s_\mu^{-1}\hat{\beta}_4], \\ \wp_\mu^{(E_\sigma)-\mu} = (-1)^{\mu+\sigma}[\frac{1}{5}\hat{\beta}_2 - (i/2)(s_\mu^{-1}\hat{\beta}_3 - s_{2\mu}^{-1}\hat{\beta}_4)], \end{cases} \quad \mu = \pm\sigma, \sigma = \frac{1}{2}, \frac{3}{2} \quad (38a)$$

$$\begin{cases} \wp_\mu^{(G_{3/2})\mu} = \frac{1}{5}\hat{e} - (i/5)(t_{2\mu}\hat{\beta}_3 - t_\mu\hat{\beta}_4), \\ \wp_\mu^{(G_{3/2})-\mu} = (-1)^{\mu-1/2}[\frac{1}{5}\hat{\beta}_2 - (i/5)(t_\mu\hat{\beta}_3 + t_{2\mu}\hat{\beta}_4)], \end{cases} \quad \mu = \pm\frac{1}{2}, \pm\frac{3}{2} \quad (38b)$$

$$\wp_\mu^{(G_{3/2})\bar{\mu}} = [2(3)^{1/2}/5]\theta_{\mu\bar{\mu}}[s_{2(\mu-\bar{\mu})}\hat{\beta}_3 - s_{\mu-\bar{\mu}}\hat{\beta}_4], \quad (\mu : \bar{\mu}) = (\pm\frac{1}{2}, \pm\frac{3}{2}),$$

where $\theta_{\mu\bar{\mu}} = \theta_{\bar{\mu}\mu}^*$ are phase factors, $\theta_{\frac{1}{2}\frac{3}{2}} = -\theta_{\frac{3}{2}\frac{1}{2}} = -\theta_{-\frac{1}{2}\frac{3}{2}} = -\theta_{-\frac{3}{2}\frac{1}{2}} = i$,

Table 3. The phase factors $\theta_{\mu\bar{\mu}}$ of $I_{5/2}$

	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{3}{2}$	$-\frac{3}{2}$	$[\frac{3}{2}]$	$[-\frac{3}{2}]$
$\frac{1}{2}$		-1	-i	i	$(i/5^{1/2})\alpha_1^*$	$(i/5^{1/2})\alpha_1$
$-\frac{1}{2}$			i	i	$-(1/5^{1/2})\alpha_1^*$	$(1/5^{1/2})\alpha_1^*$
$\frac{3}{2}$				1	$(i/5^{1/2})\alpha_2$	$(i/5^{1/2})\alpha_2^*$
$-\frac{3}{2}$					$(1/5^{1/2})\alpha_2$	$-(1/5^{1/2})\alpha_2^*$
$[\frac{3}{2}]$						$-(1/5^{1/2})\alpha_3$

$$\theta_{\mu\bar{\mu}} = -\theta_{\bar{\mu}\mu}^*. \quad \alpha_1 = 2(s_2 + is_1), \quad \alpha_2 = (1/2^{1/2})(-t_2 + it_1), \quad \alpha_3 = (8/5^{1/2})(s_2c_1^2 + is_1c_2^2).$$

$$\begin{cases} \wp_{\mu}^{(I_{5/2})\mu} = \frac{1}{5}\hat{e} + \frac{2}{5}i[s_{\mu}\hat{\beta}_3 - s_{2\mu}\hat{\beta}_4], \\ \wp_{\mu}^{(I_{5/2})-\mu} = (-1)^{\mu+1/2}[\frac{1}{5}\hat{\beta}_2 + \frac{2}{5}i(s_{2\mu}\hat{\beta}_3 + s_{\mu}\hat{\beta}_4)], \\ \mu = \pm\frac{1}{2}, \pm\frac{3}{2} \end{cases} \quad \begin{aligned} D^{(E_{1/2})}(C_{5,6}) &= \begin{bmatrix} \rho_{\frac{1}{2}} & 0 \\ 0 & \rho_{-\frac{1}{2}} \end{bmatrix}, \\ D^{(E_{1/2})}(\hat{\beta}_2) &= \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \\ D^{(E_{1/2})}(\hat{\beta}_3) &= -\frac{i}{2} \begin{bmatrix} s_1^{-1} & s_2^{-1} \\ s_2^{-1} & -s_1^{-1} \end{bmatrix}, \\ D^{(E_{1/2})}(\hat{\beta}_4) &= \frac{i}{2} \begin{bmatrix} -s_2^{-1} & s_1^{-1} \\ s_1^{-1} & s_2^{-1} \end{bmatrix}, \end{aligned} \quad (39a)$$

$$\begin{cases} \wp_{[\pm\frac{3}{2}]}^{(I_{5/2})[\pm\frac{3}{2}]} = \frac{1}{5}(\hat{e} \pm i\hat{\beta}_2) \\ \wp_{[\pm\frac{3}{2}]}^{(I_{5/2})[\mp\frac{3}{2}]} = (1/5^{1/2})\theta_{[\pm\frac{3}{2}],[\mp\frac{3}{2}]}(\hat{\beta}_3 \mp i\hat{\beta}_4) \\ \wp_{\mu}^{(I_{5/2})[\pm\frac{3}{2}]} = (1/5^{1/2})\theta_{\mu, [\pm\frac{3}{2}]}(\hat{\beta}_3 \pm i\hat{\beta}_4), \\ \mu = \pm\frac{1}{2}, \pm\frac{3}{2} \end{cases} \quad \begin{aligned} D^{(E_{3/2})}(C_{5,6}) &= \begin{bmatrix} \rho_{\frac{3}{2}} & 0 \\ 0 & \rho_{-\frac{3}{2}} \end{bmatrix}, \\ D^{(E_{3/2})}(\hat{\beta}_2) &= \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \\ D^{(E_{3/2})}(\hat{\beta}_3) &= -\frac{i}{2} \begin{bmatrix} -s_2^{-1} & s_1^{-1} \\ s_1^{-1} & s_2^{-1} \end{bmatrix}, \\ D^{(E_{3/2})}(\hat{\beta}_4) &= -\frac{i}{2} \begin{bmatrix} s_1^{-1} & s_2^{-1} \\ s_2^{-1} & -s_1^{-1} \end{bmatrix}, \end{aligned} \quad (39b)$$

$$\wp_{[\pm\frac{3}{2}]}^{(I_{5/2})\bar{\mu}} = (1/5^{1/2})\theta_{[\pm\frac{3}{2}],\bar{\mu}}(\hat{\beta}_3 \mp i\hat{\beta}_4), \quad \bar{\mu} = \pm\frac{1}{2}, \pm\frac{3}{2}, \quad (38c)$$

where the phase factors $\theta_{\mu\bar{\mu}} = -\theta_{\bar{\mu}\mu}^*$ are listed in Table 3. It is important to note that a reduced projection operator contains 4 rather than 60 terms, which represents a major simplification.

5. The $I \supset D_5 \supset C_5$ irreducible matrices

Algebraic expressions for the reduced projection operators are functions of the quantum numbers $\lambda, \mu, \bar{\mu}$ only and thus are very concise; nonetheless, they contain nearly all required information about irreducible matrix elements. Specifically, for constructing SAFs the reduced projection operators suffice; however, if one needs to find the CG coefficients, a knowledge of the irreducible matrices of the coset representatives is also required. A prescription for finding the latter follows.

Since the operator $C_{5,6} = C_{5z}$ is diagonal in the $I \supset C_5$ basis, its irreducible matrix is $D_{\mu\bar{\mu}}^{(\lambda)}(C_{5,6}) = \rho_{\mu}\delta_{\mu\bar{\mu}}$. On the other hand, according to (9b), the coefficients in front of the coset generator $\hat{\beta}_i/M_i$ in the reduced projection operators are just the complex conjugate of the matrix elements of $\hat{\beta}_i$. Therefore, from (38) one can read off the irreducible matrices of the double-coset generator $\hat{\beta}_2, \hat{\beta}_3, \hat{\beta}_4$ directly:

$$\begin{aligned} D^{(G_{3/2})}(C_{5,6}) &= \begin{bmatrix} \rho_{\frac{3}{2}} & 0 & 0 & 0 \\ 0 & \rho_{\frac{3}{2}} & 0 & 0 \\ 0 & 0 & \rho_{-\frac{3}{2}} & 0 \\ 0 & 0 & 0 & \rho_{-\frac{3}{2}} \end{bmatrix}, \\ D^{(G_{3/2})}(\hat{\beta}_2) &= \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \\ D^{(G_{3/2})}(\hat{\beta}_3) &= \frac{i}{5} \begin{bmatrix} -t_2 & 2(3)^{1/2}s_2 & 2(3)^{1/2}s_1 & t_1 \\ 2(3)^{1/2}s_2 & t_1 & -t_2 & -2(3)^{1/2}s_1 \\ 2(3)^{1/2}s_1 & -t_2 & -t_1 & 2(3)^{1/2}s_2 \\ t_1 & -2(3)^{1/2}s_1 & 2(3)^{1/2}s_2 & t_2 \end{bmatrix}, \\ D^{(G_{3/2})}(\hat{\beta}_4) &= -\frac{i}{5} \begin{bmatrix} -t_1 & 2(3)^{1/2}s_1 & -2(3)^{1/2}s_2 & -t_2 \\ 2(3)^{1/2}s_1 & -t_2 & -t_1 & 2(3)^{1/2}s_2 \\ -2(3)^{1/2}s_2 & -t_1 & t_2 & 2(3)^{1/2}s_1 \\ -t_2 & 2(3)^{1/2}s_2 & 2(3)^{1/2}s_1 & t_1 \end{bmatrix}. \end{aligned} \quad (39c)$$

Table 4. *The elements of double cosets*

j	0	1	2	3	4					
$C_{5,6}^j$	1	2	14	-15	-3					
$C_{5,6}^j \cdot 53$	53	54	49	-59	-47					
(j, k)	(0,0)	(0,1)	(0,2)	(0,3)	(0,4)	(1,0)	(1,1)	(1,2)	(1,3)	(1,4)
$C_{5,6}^j \cdot 58 \cdot C_{5,6}^k$	58	-21	-30	-28	-16	-17	-42	-32	-24	-52
$C_{5,6}^j \cdot 50 \cdot C_{5,6}^k$	50	-35	-13	-6	-44	-45	-11	-8	-41	-56
(j, k)	(2,0)	(2,1)	(2,2)	(2,3)	(2,4)	(3,0)	(3,1)	(3,2)	(3,3)	(3,4)
$C_{5,6}^j \cdot 58 \cdot C_{5,6}^k$	7	4	36	57	-40	12	26	46	37	-9
$C_{5,6}^j \cdot 50 \cdot C_{5,6}^k$	29	39	22	55	-25	31	18	60	-23	-33
(j, k)	(4,0)	(4,1)	(4,2)	(4,3)	(4,4)					
$C_{5,6}^j \cdot 58 \cdot C_{5,6}^k$	-20	-48	19	38	43					
$C_{5,6}^j \cdot 50 \cdot C_{5,6}^k$	-34	-51	27	5	10					

The eigenvalue ρ is related to the irrep label μ of C_5 by $\rho = \exp(-2\mu\pi i/5)$. The bold-face integers are indices of the group elements of I as indexed in Table 2 of Fan *et al.* (1999).

With the rows (columns) in the order of $[\frac{5}{2}], \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}, [-\frac{5}{2}]$, the matrices for the irrep $I_{5/2}$ are

$$D^{(I_{5/2})}(C_{5,6}) = \{\rho_2, \rho_3, \rho_4, \rho_{-1}, \rho_{-2}, \rho_{-3}\}_{\text{diag}}$$

$$D^{(I_{5/2})}(\hat{\beta}_2) = \begin{bmatrix} -i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i \end{bmatrix},$$

$$D^{(I_{5/2})}(\hat{\beta}_3) = \frac{i}{5^{1/2}} \begin{bmatrix} 0 & -\alpha_2 & -\alpha_1^* & -i\alpha_1^* & i\alpha_2 & -\alpha_3^* \\ -\alpha_2^* & -2s_1 & -8^{1/2}s_1 & -8^{1/2}s_2 & 2s_2 & -\alpha_2 \\ -\alpha_1 & -8^{1/2}s_1 & -2s_2 & 2s_1 & 8^{1/2}s_2 & -\alpha_1^* \\ i\alpha_1 & -8^{1/2}s_2 & 2s_1 & 2s_2 & -8^{1/2}s_1 & -i\alpha_1^* \\ -i\alpha_2^* & 2s_2 & 8^{1/2}s_2 & -8^{1/2}s_1 & 2s_1 & i\alpha_2 \\ -\alpha_3 & -\alpha_2^* & -\alpha_1 & i\alpha_1 & -i\alpha_2^* & 0 \end{bmatrix}, \tag{39d}$$

$$D^{(I_{5/2})}(\hat{\beta}_4) = -\frac{i}{5^{1/2}} \begin{bmatrix} 0 & i\alpha_2 & i\alpha_1^* & -\alpha_1^* & \alpha_2 & i\alpha_3^* \\ -i\alpha_2^* & 2s_2 & 8^{1/2}s_2 & -8^{1/2}s_1 & 2s_1 & i\alpha_2 \\ -i\alpha_1 & 8^{1/2}s_2 & -2s_1 & -2s_2 & 8^{1/2}s_1 & i\alpha_1^* \\ -\alpha_1 & -8^{1/2}s_1 & -2s_2 & 2s_1 & 8^{1/2}s_2 & -\alpha_1^* \\ \alpha_2^* & 2s_1 & 8^{1/2}s_1 & 8^{1/2}s_2 & -2s_2 & \alpha_2 \\ -i\alpha_3 & -i\alpha_2^* & -i\alpha_1 & -\alpha_1 & \alpha_2^* & 0 \end{bmatrix}, \tag{39e}$$

where the identities (24) have been used and

$$\alpha_1 = 2(s_2 + is_1), \quad \alpha_2 = (1/2^{1/2})(-t_2 + it_1),$$

$$\alpha_3 = (8/5^{1/2})(s_2c_1^2 + is_1c_2^2).$$

Chen & Fan (1998c) show that when calculating CG coefficients with the reduced projection operator only the irreducible matrices of the above double-coset representatives are required. If one needs the irreducible matrices of other elements, they can be obtained through the following simple formulas:

$$D_{\mu\bar{\mu}}^{(\lambda)}(C_{5,6}^j \hat{\beta}_2) = \rho_{\mu}^j D_{\mu\bar{\mu}}^{(\lambda)}(\hat{\beta}_2),$$

$$D_{\mu\bar{\mu}}^{(\lambda)}(C_{5,6}^j \hat{\beta}_3 C_{5,6}^k) = \rho_{\mu}^j D_{\mu\bar{\mu}}^{(\lambda)}(\hat{\beta}_3) \rho_{\bar{\mu}}^k, \tag{40}$$

$$D_{\mu\bar{\mu}}^{(\lambda)}(C_{5,6}^j \hat{\beta}_4 C_{5,6}^k) = \rho_{\mu}^j D_{\mu\bar{\mu}}^{(\lambda)}(\hat{\beta}_4) \rho_{\bar{\mu}}^k.$$

Using the group table of I^\dagger , we can obtain the pair of indexes (j, k) for each element of I^\dagger , as shown in Table 4. Equations (39) and (40) give the algebraic expressions of the irreducible matrix elements.

6. The $I \supset D_5 \supset C_5$ SAFs

We now derive algebraic expressions for SAFs, which are functions of the angular momentum j , the quantum numbers λ, μ and the multiplicity label \bar{m} . As shown in Fan *et al.* (1999), the SAFs can be obtained by applying the reduced projection operator to a trial state $|j\bar{m}\rangle$,

$$\psi_{\mu}^{(\lambda)\bar{m}} = \wp_{\mu}^{(\lambda)\bar{\mu}} |j\bar{m}\rangle, \tag{41a}$$

where magnetic quantum number conservation rules apply,

$$\bar{m} \doteq \bar{\mu}, \quad m \doteq \mu. \tag{41b}$$

Here, $\bar{m} \doteq \bar{\mu}$ means $\bar{m} = \bar{\mu} \pmod{5}$ and for each irrep we need only one set of the reduced projection operators with a specific intrinsic quantum number $\bar{\mu}$, which is chosen to be $\frac{1}{2}$ for all irreps except the $E_{3/2}$ in which case $\bar{\mu} = \frac{3}{2}$, that is,

$$\wp_{\mu}^{(E_{1/2})\frac{1}{2}}, \quad \wp_{\mu}^{(E_{3/2})\frac{3}{2}}, \quad \wp_{\mu}^{(G_{3/2})\frac{1}{2}}, \quad \wp_{\mu}^{(I_{5/2})\frac{1}{2}}. \tag{41c}$$

Using the D function from Rose (1957) and the Euler angles for the coset representatives listed in Table 2 of Fan *et al.* (1999), we have that

$$\hat{\beta}_2 |j\bar{m}\rangle = (-1)^{j-\bar{m}} |j-\bar{m}\rangle,$$

$$\hat{\beta}_3 |j\bar{m}\rangle = \sum_m \exp(-i\bar{m}\pi) d_{m\bar{m}}^j(\beta_3) |jm\rangle, \tag{41d}$$

$$\hat{\beta}_4 |j\bar{m}\rangle = \sum_m \exp(-im\pi) d_{m\bar{m}}^j(\beta_4) |jm\rangle,$$

where $\beta_3 = \pi - \omega$ and $\beta_4 = \omega$.

From (41a)–(41d), we obtain the unnormalized $I \supset D_5 \supset C_5$ d-v SAFs:

Table 5. The multiplicity τ_λ^j of the irrep λ of the group I in the subduced rep $D^j \downarrow I$

j	A	F_1	F_2	G	H	j	$E_{1/2}$	$E_{3/2}$	$G_{3/2}$	$I_{5/2}$
0	1					1/2	1			
1		1				3/2			1	
2					1	5/2				1
3			1	1		7/2		1		1
4				1	1	9/2			1	1
5		1	1		1	11/2	1		1	1
6	1	1		1	1	13/2	1	1	1	1
7		1	1	1	1	15/2			1	2
8			1	1	2	17/2		1	1	2
9		1	1	2	1	19/2	1	1	1	2
10	1	1	1	1	2	21/2	1		2	2
11		2	1	1	2	23/2	1	1	2	2
12	1	1	1	2	2	25/2	1	1	1	3
13		1	2	2	2	27/2		1	2	3
14		1	1	2	3	29/2	1	1	2	3

$D^j = \text{reg} - D^{29-j}$, $j = 15, 31/2, \dots, 28, 57/2, 29$. $D^{30n+l} = n \text{reg} + D^l$, $l = 0, 1, 2, \dots, 29$, $\text{reg} = A + 3F_1 + 3F_2 + 4G + 5H$.
 $D^{30n+l} = n \text{reg} + D^l$, $j = 1/2, 3/2, \dots, 59/2$, $D^{59/2} = \text{reg} = 2E_{1/2} + 2E_{3/2} + 4G_{3/2} + 6I_{5/2}$.

(i) Two-dimensional irreps

$$\begin{aligned}
 \psi_\mu^{(E_\mu)\bar{m}} &= |j\bar{m}\rangle + \frac{5}{2} \sum_{m \neq \mu} [(-1)^{\bar{m}-1/2} s_{2\mu}^{-1} d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m-1/2} s_\mu^{-1} d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \quad \mu = \frac{1}{2}, \frac{3}{2}, \quad (42) \\
 \psi_{-\mu}^{(E_\mu)\bar{m}} &= (-1)^{j-\bar{m}} |j-\bar{m}\rangle - \frac{5}{2} \sum_{m \neq -\mu} [(-1)^{\bar{m}-1/2} s_\mu^{-1} d_{m\bar{m}}^j(\beta_3) \\
 &\quad - (-1)^{m-1/2} s_{2\mu}^{-1} d_{m\bar{m}}^j(\beta_4)] |jm\rangle.
 \end{aligned}$$

(ii) Four-dimensional irrep

$$\begin{aligned}
 \psi_{\frac{1}{2}}^{(G_{3/2})\bar{m}} &= |j\bar{m}\rangle - \sum_{m \neq 1/2} [(-1)^{\bar{m}-1/2} t_1 d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m-1/2} t_2 d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \\
 \psi_{-\frac{1}{2}}^{(G_{3/2})\bar{m}} &= (-1)^{j+\bar{m}} |j-\bar{m}\rangle + \sum_{m \neq -1/2} [(-1)^{\bar{m}-1/2} t_2 d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m+1/2} t_1 d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \quad (43a) \\
 \psi_\mu^{(G_{3/2})\bar{m}} &= \sum_{m \neq \mu} [(-1)^{\bar{m}+1/2} s_{2\mu-1} d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m-1/2} s_{\mu-1/2} d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \quad \mu = \pm \frac{3}{2}.
 \end{aligned}$$

(iii) Six-dimensional irrep

$$\begin{aligned}
 \psi_{\frac{1}{2}}^{(I_{5/2})\bar{m}} &= |j\bar{m}\rangle + 2 \sum_{m \neq 1/2} [(-1)^{\bar{m}-1/2} s_2 d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m+1/2} s_1 d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \\
 \psi_{-\frac{1}{2}}^{(I_{5/2})\bar{m}} &= (-1)^{j-\bar{m}} |j-\bar{m}\rangle - 2 \sum_{m \neq -1/2} [(-1)^{\bar{m}-1/2} s_1 d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m-1/2} s_2 d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \quad (43b) \\
 \psi_\mu^{(I_{5/2})\bar{m}} &= (-1)^{\mu-1/2} \sum_{m \neq \mu} [(-1)^{\bar{m}-1/2} s_{2\mu+1} d_{m\bar{m}}^j(\beta_3) \\
 &\quad - (-1)^{m-1/2} s_{\mu+1/2} d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \quad \mu = \pm \frac{3}{2}, \\
 \psi_{[\pm \frac{3}{2}]}^{(I_{5/2})\bar{m}} &= (1/2^{1/2}) [\psi_{\frac{3}{2}}^{(I_{5/2})\bar{m}} \pm i \psi_{-\frac{3}{2}}^{(I_{5/2})\bar{m}}],
 \end{aligned}$$

where

$$\begin{aligned}
 \psi_{\frac{3}{2}}^{(I_{5/2})\bar{m}} &= \sum_{m \neq 5/2} [(-1)^{\bar{m}-1/2} s_2 d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m-1/2} s_1 d_{m\bar{m}}^j(\beta_4)] |jm\rangle, \\
 \psi_{-\frac{3}{2}}^{(I_{5/2})\bar{m}} &= \sum_{m \neq -5/2} [(-1)^{\bar{m}-1/2} s_1 d_{m\bar{m}}^j(\beta_3) \\
 &\quad + (-1)^{m+1/2} s_2 d_{m\bar{m}}^j(\beta_4)] |jm\rangle
 \end{aligned} \quad (44)$$

are two real functions. As will be shown later [see equations (47) and (48)], these functions form the $SO_3 \downarrow I$ irreducible basis. Note that except for the irrep $I_{5/2}$, the $I \supset C_s$ SAFs and $SO_3 \downarrow I$ SAFs are identical for all irreps (including all s-v irreps, and the d-v irreps $E_{1/2}$, $E_{3/2}$ and $G_{3/2}$).

7. The multiplicity problem and symmetries of the SAFs

In (42)–(43b), the quantum \bar{m} serves naturally as the multiplicity label of the irrep λ in the subduced rep $D^j \downarrow I$, and its possible values are decided by (41b) and (41c), that is

$$\bar{m} \doteq \begin{cases} \frac{1}{2}, & \text{for } E_{1/2}, G_{3/2}, I_{5/2} \\ \frac{3}{2}, & \text{for } E_{3/2}. \end{cases}$$

In general, SAFs $\psi_\mu^{(\lambda)\bar{m}}$ with different \bar{m} may be neither orthogonal nor linearly independent. When an irrep λ occurs only once in D^j , \bar{m} may take any permissible value. The results with different \bar{m} differ at most by an overall phase. When an irrep λ occurs τ times, we need to let \bar{m} taking τ different values, $\bar{m} = \bar{\mu}, \bar{\mu} + 5, \bar{\mu} - 5, \dots$ According to our experience, the τ sets of SAFs $\psi_\mu^{(\lambda)\bar{m}}$ are always linearly independent, though not orthogonal in \bar{m} . In practical calculation, as a check we evaluate the determinant of the $\tau \times \tau$ overlap matrix,

Table 6. *The d-v SAFs for $I \supset D_5 \supset C_5$ [$I_{5/2} \pm \frac{5}{2}$] are $SO_3 \downarrow I$ SAFs, see equations (43b) and (44)*

$$j = \frac{1}{2} \quad \bar{m} = \frac{1}{2} \quad |E_{1/2} \mu\rangle = |\frac{1}{2} \mu\rangle, \quad \mu = \pm \frac{1}{2}, \quad j = \frac{3}{2} \quad \bar{m} = \frac{1}{2} \quad |G_{3/2} \mu\rangle = |\frac{3}{2} \mu\rangle, \quad \mu = \pm \frac{1}{2}, \pm \frac{3}{2}$$

$$j = \frac{5}{2} \quad \bar{m} = \frac{1}{2} \quad |I_{5/2} \mu\rangle = |\frac{5}{2} \mu\rangle, \quad \pm \frac{1}{2}, \pm \frac{3}{2}, \pm \frac{5}{2}$$

$$j = \frac{7}{2} \quad \bar{m} = -\frac{7}{2}$$

$$|E_{3/2} \frac{3}{2}\rangle = [(2 \times 3 \times 5)^{1/2} / (2 \times 5)] |\frac{7}{2} - \frac{7}{2}\rangle + [(2 \times 5 \times 7)^{1/2} / (2 \times 5)] |\frac{7}{2} \frac{3}{2}\rangle$$

$$|E_{3/2} -\frac{3}{2}\rangle = [(2 \times 5 \times 7)^{1/2} / (2 \times 5)] |\frac{7}{2} - \frac{3}{2}\rangle - [(2 \times 3 \times 5)^{1/2} / (2 \times 5)] |\frac{7}{2} \frac{3}{2}\rangle$$

$$\bar{m} = \frac{1}{2}$$

$$|I_{5/2} \frac{5}{2}\rangle = -[7 / (5 \times 2^{1/2})] |\frac{7}{2} - \frac{5}{2}\rangle + [1 / (5 \times 2^{1/2})] |\frac{7}{2} \frac{5}{2}\rangle$$

$$|I_{5/2} \frac{3}{2}\rangle = [(2 \times 5 \times 7)^{1/2} / (2 \times 5)] |\frac{7}{2} - \frac{7}{2}\rangle - [(2 \times 3 \times 5)^{1/2} / (2 \times 5)] |\frac{7}{2} \frac{3}{2}\rangle$$

$$|I_{5/2} \frac{1}{2}\rangle = |\frac{7}{2} \frac{1}{2}\rangle$$

$$|I_{5/2} -\frac{1}{2}\rangle = -|\frac{7}{2} - \frac{1}{2}\rangle$$

$$|I_{5/2} -\frac{3}{2}\rangle = [(2 \times 3 \times 5)^{1/2} / (2 \times 5)] |\frac{7}{2} - \frac{3}{2}\rangle + [(2 \times 5 \times 7)^{1/2} / (2 \times 5)] |\frac{7}{2} \frac{3}{2}\rangle$$

$$|I_{5/2} -\frac{5}{2}\rangle = -[1 / (5 \times 2^{1/2})] |\frac{7}{2} - \frac{5}{2}\rangle - [7 / (5 \times 2^{1/2})] |\frac{7}{2} \frac{5}{2}\rangle$$

$$j = \frac{15}{2} \quad \bar{m} = -\frac{9}{2}$$

$$|I_{5/2} \frac{1}{2}\rangle = [2(5 \times 29)^{1/2} / 5^2] |\frac{15}{2} - \frac{9}{2}\rangle + [3(5 \times 7 \times 11 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} \frac{1}{2}\rangle + [3(3 \times 5 \times 13 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} \frac{17}{2}\rangle$$

$$|I_{5/2} -\frac{1}{2}\rangle = [3(3 \times 5 \times 13 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{17}{2}\rangle - [3(5 \times 7 \times 11 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{1}{2}\rangle + [2(5 \times 29)^{1/2} / 5^2] |\frac{15}{2} \frac{9}{2}\rangle$$

$$|I_{5/2} \frac{3}{2}\rangle = -[3^3(2 \times 3 \times 5 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{7}{2}\rangle - [19(2 \times 5 \times 11 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} \frac{3}{2}\rangle$$

$$+ [(2 \times 3 \times 5 \times 7 \times 13 \times 29)^{1/2} / (5^2 \times 29)] |\frac{15}{2} \frac{13}{2}\rangle$$

$$|I_{5/2} -\frac{3}{2}\rangle = [(2 \times 3 \times 5 \times 7 \times 13 \times 29)^{1/2} / (5^2 \times 29)] |\frac{15}{2} - \frac{13}{2}\rangle + [19(2 \times 5 \times 11 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{3}{2}\rangle$$

$$- [3^3(2 \times 3 \times 5 \times 29)^{1/2} / (2 \times 5^2 \times 29)] |\frac{15}{2} \frac{7}{2}\rangle$$

$$|I_{5/2} \frac{5}{2}\rangle = [11(2 \times 5 \times 7 \times 13 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{5}{2}\rangle + [17(2 \times 3 \times 5 \times 11 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{9}{2}\rangle$$

$$- [11(2 \times 3 \times 5 \times 11 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} \frac{5}{2}\rangle - [7(2 \times 5 \times 7 \times 13 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} \frac{13}{2}\rangle$$

$$|I_{5/2} -\frac{5}{2}\rangle = -[7(2 \times 5 \times 7 \times 13 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{13}{2}\rangle + [11(2 \times 3 \times 5 \times 11 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} - \frac{5}{2}\rangle$$

$$+ [17(2 \times 3 \times 5 \times 11 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} \frac{9}{2}\rangle - [11(2 \times 5 \times 7 \times 13 \times 29)^{1/2} / (2^2 \times 5^2 \times 29)] |\frac{15}{2} \frac{13}{2}\rangle$$

$$\bar{m} = \frac{1}{2}$$

$$|I_{5/2} \frac{1}{2}\rangle = [(3 \times 5 \times 7 \times 11)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} - \frac{9}{2}\rangle + [2^2(3 \times 5)^{1/2} / 5^2] |\frac{15}{2} \frac{1}{2}\rangle - [(5 \times 7 \times 11 \times 13)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} \frac{17}{2}\rangle$$

$$|I_{5/2} -\frac{1}{2}\rangle = -[(5 \times 7 \times 11 \times 13)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} - \frac{17}{2}\rangle - [2^2(3 \times 5)^{1/2} / 5^2] |\frac{15}{2} - \frac{1}{2}\rangle + [(3 \times 5 \times 7 \times 11)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} \frac{9}{2}\rangle$$

$$|I_{5/2} \frac{3}{2}\rangle = -[7(2 \times 5 \times 7 \times 11)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} - \frac{7}{2}\rangle + [(2 \times 3 \times 5 \times 7)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} \frac{3}{2}\rangle - [(2 \times 5 \times 11 \times 13)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} \frac{13}{2}\rangle$$

$$|I_{5/2} -\frac{3}{2}\rangle = -[(2 \times 5 \times 11 \times 13)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} - \frac{13}{2}\rangle - [(2 \times 3 \times 5 \times 7)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} - \frac{3}{2}\rangle - [7(2 \times 5 \times 7 \times 11)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} \frac{7}{2}\rangle$$

$$|I_{5/2} \frac{5}{2}\rangle = [(2 \times 3 \times 5 \times 11 \times 13)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} - \frac{5}{2}\rangle + [11(2 \times 5 \times 7)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} - \frac{9}{2}\rangle + [3(2 \times 5 \times 7)^{1/2} / (2 \times 5^2)] |\frac{15}{2} \frac{5}{2}\rangle$$

$$+ [(2 \times 3 \times 5 \times 11 \times 13)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} \frac{15}{2}\rangle$$

$$|I_{5/2} -\frac{5}{2}\rangle = [(2 \times 3 \times 5 \times 11 \times 13)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} - \frac{15}{2}\rangle - [3(2 \times 5 \times 7)^{1/2} / (2 \times 5^2)] |\frac{15}{2} - \frac{5}{2}\rangle + [11(2 \times 5 \times 7)^{1/2} / (2^3 \times 5^2)] |\frac{15}{2} \frac{9}{2}\rangle$$

$$- [(2 \times 3 \times 5 \times 11 \times 13)^{1/2} / (2^2 \times 5^2)] |\frac{15}{2} \frac{15}{2}\rangle$$

$$j = \frac{17}{2}, \quad \bar{m} = -\frac{17}{2}$$

$$|E_{3/2} \frac{3}{2}\rangle = [2(3 \times 5 \times 13)^{1/2} / (3 \times 5^2)] |\frac{17}{2} - \frac{17}{2}\rangle - [(3 \times 5 \times 7 \times 17)^{1/2} / (3 \times 5^2)] |\frac{17}{2} - \frac{7}{2}\rangle + [(2 \times 3 \times 5 \times 11 \times 17)^{1/2} / (2 \times 3 \times 5^2)] |\frac{17}{2} \frac{3}{2}\rangle$$

$$- [(2 \times 3 \times 5 \times 13 \times 17)^{1/2} / (2 \times 3 \times 5^2)] |\frac{17}{2} \frac{13}{2}\rangle$$

$$|E_{3/2} -\frac{3}{2}\rangle = -[(2 \times 3 \times 5 \times 13 \times 17)^{1/2} / (2 \times 3 \times 5^2)] |\frac{17}{2} - \frac{13}{2}\rangle - [(2 \times 3 \times 5 \times 11 \times 17)^{1/2} / (2 \times 3 \times 5^2)] |\frac{17}{2} - \frac{3}{2}\rangle$$

$$- [(3 \times 5 \times 7 \times 17)^{1/2} / (3 \times 5^2)] |\frac{17}{2} \frac{7}{2}\rangle - [2(3 \times 5 \times 13)^{1/2} / (3 \times 5^2)] |\frac{17}{2} \frac{17}{2}\rangle$$

$$\bar{m} = -\frac{9}{2}$$

$$|G_{3/2} \frac{1}{2}\rangle = [(5 \times 7 \times 11)^{1/2} / 5^2] |\frac{17}{2} - \frac{9}{2}\rangle + [(2 \times 5 \times 13)^{1/2} / 5^2] |\frac{17}{2} \frac{1}{2}\rangle - [(2 \times 5 \times 11)^{1/2} / 5^2] |\frac{17}{2} \frac{17}{2}\rangle$$

$$|G_{3/2} -\frac{1}{2}\rangle = -[(2 \times 5 \times 11)^{1/2} / 5^2] |\frac{17}{2} - \frac{17}{2}\rangle - [(2 \times 5 \times 13)^{1/2} / 5^2] |\frac{17}{2} - \frac{1}{2}\rangle + [(5 \times 7 \times 11)^{1/2} / 5^2] |\frac{17}{2} \frac{9}{2}\rangle$$

$$|G_{3/2} \frac{3}{2}\rangle = -[2(3 \times 11 \times 17)^{1/2} / (3 \times 5^2)] |\frac{17}{2} - \frac{17}{2}\rangle - [(3 \times 7 \times 11 \times 13)^{1/2} / (3 \times 5^2)] |\frac{17}{2} - \frac{7}{2}\rangle - [2(2 \times 3 \times 13)^{1/2} / (3 \times 5^2)] |\frac{17}{2} \frac{3}{2}\rangle$$

$$+ [(2 \times 3 \times 11)^{1/2} / (3 \times 5^2)] |\frac{17}{2} \frac{13}{2}\rangle$$

$$|G_{3/2} -\frac{3}{2}\rangle = [(2 \times 3 \times 11)^{1/2} / (3 \times 5^2)] |\frac{17}{2} - \frac{13}{2}\rangle + [2(2 \times 3 \times 13)^{1/2} / (3 \times 5^2)] |\frac{17}{2} - \frac{3}{2}\rangle - [(3 \times 7 \times 11 \times 13)^{1/2} / (3 \times 5^2)] |\frac{17}{2} \frac{7}{2}\rangle$$

$$+ [2(3 \times 11 \times 17)^{1/2} / (3 \times 5^2)] |\frac{17}{2} \frac{17}{2}\rangle$$

$$\det |\langle \psi_{\mu}^{(\lambda)\bar{m}} | \psi_{\mu}^{(\lambda)\bar{m}'} \rangle|,$$

for any given value of μ . If it is nonzero, then the τ sets of SAFs $\psi_{\mu}^{(\lambda)\bar{m}}$ are linearly independent. We checked the cases with j up to $59/2$ and no example of linear dependence is found. To find numerical results from the algebraic expressions, the multiplicity τ_{λ}^j for the occurrence of the irrep λ of I in the subduced representation

$D^j \downarrow I$ is calculated first by using the character theory and is used as a control parameter for the calculation. An orthogonal procedure is not included; to do so would lose the simplicity of the algebraic expressions for SAFs. The table of the multiplicity τ_{λ}^j is given in Table 5.

With the algebraic expressions in hand, it is very easy to find the exact numerical expression of the SAFs $\psi_{\mu}^{(\lambda)\bar{m}}$ for any j with the help of some software such as *Maple*

(Char *et al.*, 1992). Part of the d-v $I \supset D_5 \supset C_5$ SAFs are listed in Table 6. They are all linearly independent, but not orthogonal with respect to \bar{m} . Our result are identical with the tables given by Damhus *et al.* (1984, p. 439) for $j = \frac{1}{2} - \frac{9}{2}$ for the multiplicity-free case.

From (42)–(44) and using properties of $d_{m\bar{m}}^j(\beta)$ as given in Rose (1957), we can derive the following symmetries for the SAFs:

$$\begin{aligned} \langle jm | \psi_{\mu}^{(E_{\mu})\bar{m}} \rangle &= (-1)^{j-m} \langle j-m | \psi_{-\mu}^{(E_{\mu})\bar{m}} \rangle, & \mu &= \frac{1}{2}, \frac{3}{2}, \\ \langle jm | \psi_{\mu}^{(G_{3/2})\bar{m}} \rangle &= (-1)^{j+m+\mu-1/2} \langle j-m | \psi_{-\mu}^{(G_{3/2})\bar{m}} \rangle, & \mu &= \frac{1}{2}, \frac{3}{2}, \\ \langle jm | \psi_{\mu}^{(I_{5/2})\bar{m}} \rangle &= (-1)^{j-m+\mu-1/2} \langle j-m | \psi_{-\mu}^{(I_{5/2})\bar{m}} \rangle, & \mu &= \frac{1}{2}, \frac{3}{2}, \frac{5}{2}. \end{aligned} \quad (45)$$

Clearly, the SAFs have high symmetry and the symmetry is independent of the multiplicity label \bar{m} .

8. Discussion and summary

The projection-operator method is often quoted as extremely difficult for large-order groups. By using reduced projection operators, the projection-operator method becomes extremely simple and powerful. This has enabled us to find algebraic expressions for SAFs of I . Another interesting point is that, among the 60 elements of I , only the 4 double-coset representatives play a key role. The role played by all the other remaining elements is merely to ensure that the magnetic quantum number conservation rules are satisfied for the initial (trial) state and for the final (projected) state.

McLellian (1961) used the subduction method to derive the irreducible matrices of the group I . The $D^j \downarrow I$ subduced representation is irreducible for $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, corresponding to the irreps $E_{1/2}, G_{3/2}, I_{5/2}$. The irreducible basis obtained by the subduction method is called the $SO_3 \downarrow I$ irreducible basis, and is labelled by (λ, m) or (Γ, m) , where m is the quantum number of j_z . McLellian also gives the irreducible matrices of the generator $\hat{\beta}_4 = C_{2,5}$, which is denoted by the symbol C in the McLellian (1961) article. Notice that McLellian used $\rho_m = \exp(2\pi m/5i)$ and his quantum number m is equivalent to our $-\mu$. The relationship between the $SO_3 \downarrow I$ irreducible matrix in McLellian (1961), denoted as $D^{(\lambda)}(R_a)$, and our $D^{(\lambda)}(R_a)$ is

$$D^{(\lambda)}(R_a) = U^{-1} D^{(\lambda)'}(R_a) U, \quad (46)$$

where U are

$$\begin{aligned} U^{E_{1/2}} &= \{1 \quad i\}_{\text{diag}}, & U^{E_{3/2}} &= \{1 \quad i\}_{\text{diag}} \\ U^{G_{3/2}} &= \{1 \quad 1 \quad i \quad -i\}_{\text{diag}} \\ U^{I_{5/2}} &= \begin{pmatrix} (1/2^{1/2}) & 0 & 0 & 0 & 0 & -(1/2^{1/2}) \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & -i & 0 \\ (1/2^{1/2}) & 0 & 0 & 0 & 0 & (1/2^{1/2}) \end{pmatrix}, \end{aligned} \quad (47)$$

where the rows of the matrix $U^{I_{5/2}}$ are of order $m = \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}$.

The corresponding irreducible basis denoted by ψ_{μ}^{λ} is given by

$$\psi_m^{\lambda} = \sum_{\mu} U_{m\mu}^* \psi_{\mu}^{\lambda}. \quad (48)$$

However, the irreducible bases ψ_m^{λ} differ from the McLellian basis by phase factors owing to the different choice of the coordinate axes. From (43b), (47) and (48), we know that $\psi_{\pm 5/2}^{(I_{5/2})\bar{m}}$ in (44) are the $SO_3 \downarrow I$ irreducible basis.

The $I \supset D_5 \supset C_5$ SAFs obtained in this paper and those derived by Butler (1981) are identical up to phases; and all are real except for the irrep $I_{5/2}$ associated with the components $\mu = [\pm \frac{5}{2}]$. The latter is in contrast with McLellian (1961) who gives SAFs that are all complex.

In summary, the algebraic expressions (38) for the reduced projection operators and equations (42)–(44) for SAFs in the group chain $I \supset D_5 \supset C_5$ have been derived using a double-induced technique in an *ab initio* way. The algebraic expressions for the former are only functions of the quantum numbers $(\lambda, \mu, \bar{\mu})$, and those for the latter are functions of only the quantum numbers $(j, \lambda, \mu, \bar{m})$ with \bar{m} serving as the multiplicity label. With the algebraic expression of SAFs available, the symmetries of SAFs were found. Combining this study for the d-v case with the previous one for the s-v case, a complete solution for the SAF problem of the icosahedral group I is achieved (for the cases with multiplicity, the SAFs are determined only up to an equivalence transformation).

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