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Symmetry functions adapted to the subgroup chain $U(7) \supset SO(7) \supset G_2 \supset SO(3) \supset G$

Wen Zhenyi,[1] Wang Yubin,[1] Dou Yusheng,[2] and Liu Zhaomeng[2]
[1]Institute of Modern Physics, and [2]Department of Chemistry, Northwest University, Xian, Shaanxi, People's Republic of China

Summary. In this paper the Lie algebra technique is used to construct symmetry functions adapted to the subgroup chain $U(7) \supset SO(7) \supset G_2 \supset SO(3) \supset G$, which is one of symmetry group chains appearing in the weak ligand field scheme for f^N ions. The functions are expressed in terms of the Gelfand states.

Key words: Symmetry adapted functions — Unitary group approach — Ligand field theory

1. Introduction

In both atomic spectroscopy and ligand field theory it is important to construct symmetry functions adapted to a given subgroup chain. In the case of an f-shell, one of the subgroup chains is

$$U(7) \supset SO(7) \supset G_2 \supset SO(3) \supset G. \tag{1}$$

This subgroup chain, except for the finite group G, was first introduced by Racah [1]. In order to construct the symmetry functions Racah defined the coefficient of fractional parentage (CFP). Although, by using the Wigner–Eckart theorem, it may not be necessary to explicitly construct the symmetry functions in Racah's procedure, many-electron reduced matrix elements have to be determined. The latter involves complex CFP factors and it therefore requires some rather elaborate calculations [2, 3]. Thus, it is advisable to suggest an efficient approach different from Racah's. The unitary group approach (UGA) is one of this type.

In the UGA a completely antisymmetric function is expanded in terms of the Gelfand basis rather than Slater determinants. The possibility of the expansion was first pointed out by Moshinsky [4] and used for constructing atomic term functions by Harter [5]. This approach was then extended and developed in works of Drake et al. [6, 7], Patterson et al. [8], Kent and Schlesinger [9], and Wen [10]. These works, however, did not consider the adaptation to symmetries of $SO(7)$ and G_2. Thus their approach leads to repetitions of term labellings and also requires solution of linear equation sets of high orders. For example, in their approach linear equations of orders of 58 and 48 respectively must be solved in order to obtain 10 ^{2}F and 10 ^{2}G term functions of an f^7 system. Orders of linear equation sets and repetitions of term labellings will be greatly reduced if the symmetry adaption to $SO(7)$ and G_2 is taken into account. The aim of this paper is to develop an algebraic technique for producing symmetry adapted term functions, i.e. the functions adapted to the group chain (1). We shall use the triplets of an f^4 system to illustrate the method.

2. Notations

Since the GUA has been discussed in detail in [11, 12] we only cite some useful notation and conclusions from these references. The basic brick of the GUA is the Gelfand basis, the canonical basis set for $U(n)$ irreducible representation (irrep). There are a number of schemes to label a Gelfand state. For systems of electrons a concise labelling is Paldus' ABC tableau, an $n \times 3$ integer matrix, in which $A \equiv [a_n, a_{n-1}, \ldots, a_1]^+$, $B \equiv [b_n, b_{n-1}, \ldots, b_1]^+$ and $C \equiv [c_n, c_{n-1}, \ldots, c_1]^+$, where a_r, b_r and c_r record the number of orbitals which are doubly-, singly- and un-occupied in the first r orbitals. A more concise labelling is the step vector $|(d_r)\rangle \equiv |(d_1 d_2 \cdots d_n)\rangle$, where d_r (called step number) is defined as

$$d_r = 3\Delta a_r + \Delta b_r. \tag{2}$$

Here

$$\begin{aligned} \Delta a_r &= a_r - a_{r-1}, \\ \Delta b_r &= b_r - b_{r-1}, \qquad r = 1, 2, \ldots, n \end{aligned} \tag{3}$$

and

$$a_0 = b_0 = 0.$$

Another important concept in the GUA is the generator E_{ij}, which satisfies the commutation relation,

$$[E_{ij}, E_{kl}] = \delta_{jk} E_{il} - \delta_{il} E_{kj}. \tag{4}$$

Under action of a generator E_{ij}, a Gelfand state is transformed according to

$$E_{ij} |(d_r)\rangle = \sum_{(d_r')} |(d_r')\rangle\langle(d_r')| E_{ij} |(d_r)\rangle. \tag{5}$$

Duch and Karwowski [13], Robb and Niazi [14] and one of the authors [15] have suggested some algorithms by which the states appearing in the right-hand side of Eq. (5) can be easily found. In this paper we only need the Paldus formula for elementary generators $E_{r+1,r}$ and $E_{r,r+1}$ [16]. We may rewrite the Paldus formula as follows:

$$\begin{aligned} E_{r+1,r}&|(d_1, \ldots, d_r, d_{r+1}, \ldots, d_n)\rangle \\ &= \left[\frac{b_r(b_r+1)}{(b_{r-1}+1)(b_{r+1}+1)}\right]^{1/2} |(d_1, \ldots, d_r - 1, d_{r+1}+1, \ldots, d_n)\rangle \\ &+ \left[\frac{(b_r+1)(b_r+2)}{(b_{r-1}+1)(b_{r+1}+1)}\right]^{1/2} |(d_1, \ldots, d_r - 2, d_{r+1}+2, \ldots, d_n)\rangle. \end{aligned} \tag{6}$$

It can be verified that the first term is different from zero if $d_r d_{r+1} = 10$, 12, 32 and 30, and the second one is different from zero if $d_r d_{r+1} = 20$, 21, 31 and 30.

The one-electron functions used in this paper are $|3m\rangle$, where $m = 3$, 2, 1, 0, -1, -2, and -3 correspond, respectively, to the orbital index $i = 1, 2, \ldots, 7$. The Gelfand states of $U(7)$ can be built from these orbitals, but we do not need their explicit form. The generators of $U(7)$ are E_{ij} $(i, j = 1, \ldots, 7)$.

3. Algebraic bases of $SO(7)$, G_2 and $SO(3)$

In this section, we shall choose linear combinations of E_{ij} to construct generators of $SO(7)$, G_2 and $SO(3)$. These generators serve as algebraic bases of the groups. As is well known [17], $SO(7)$, G_2 and $SO(3)$ are semisimple Lie groups and their generators form corresponding semisimple algebras. For any semisimple algebra there are two kinds of generators: the maximal commuting subalgebra consisting of weight operators $H = \{H_1, H_2, \ldots, H_l\}$, called the Cartan subalgebra, and the remaining ones, which are eigenvectors of H_i, are called root operators. The root operators can be divided according to their eigenvalues or roots α. The dimension l of a Cartan subalgebra is called the rank of the semisimple algebra. The ranks of $SO(7)$, G_2 and $SO(3)$ are 3, 2 and 1, respectively. Dynkin [18] has proved that in the root set of a semisimple algebra there is a subset of exactly l roots, in terms of which a root can be expressed as

$$\alpha = \sum_{j=1}^{l} k_j \alpha_j, \tag{7}$$

where k_j are all real and rational. A root is said to be positive with respect to a chosen basis set α_j if the first non-vanishing coefficient in Eq. (7) is positive. There are obviously l positive roots, each of which has a coefficient of 1 and the other of zero. This is a so-called simple root set. If the simple root set is chosen as the basis the coefficients in Eq. (7) will either be all positive or all negative. The simple root set (its dimension, length of each root and the angle made by two roots) identifies the semisimple algebra. A diagrammatic classification of semisimple algebras has been done by Dynkin [18]. The Dynkin diagrams for $SO(7)$ and G_2 are shown in Tables 1 and 2, respectively.

Now let us find the generators of $SO(7)$, G_2 and $SO(3)$. It should be noted that different authors give different definitions of the generators of these groups.

Table 1. The algebraic basis of $SO(7)$

Weight operators	$H_1 = E_{11} - E_{77}$	
	$H_2 = E_{22} - E_{66}$	
	$H_3 = E_{33} - E_{55}$	
Dynkin diagram	⊙—⊙=● α_1 α_2 α_3	
	$E_{\alpha_1} = E_{12} + E_{67}$	$(1, -1, 0)$
	$E_{\alpha_2} = E_{23} + E_{56}$	$(0, 1, -1)$
	$E_{\alpha_3} = E_{34} + E_{45}$	$(0, 0, 1)$
	$E_{\alpha_1+\alpha_2} = E_{13} - E_{57}$	$(1, 0, -1)$
	$E_{\alpha_2+\alpha_3} = E_{24} - E_{46}$	$(0, 1, 0)$
	$E_{\alpha_2+2\alpha_3} = E_{25} + E_{36}$	$(0, 1, 1)$
	$E_{\alpha_1+\alpha_2+\alpha_3} = E_{14} + E_{47}$	$(1, 0, 0)$
	$E_{\alpha_1+\alpha_2+2\alpha_3} = E_{15} - E_{37}$	$(1, 0, 1)$
	$E_{\alpha_1+2\alpha_2+2\alpha_3} = E_{16} + E_{27}$	$(1, 1, 0)$

Table 2. The algebraic basis of G_2

Weight operators	$H'_1 = E_{11} + E_{33} - E_{55} - E_{77}$	
	$H'_2 = E_{22} - E_{33} + E_{55} - E_{66}$	
Dynkin diagram	⊙=● α β	
	$E_\alpha = E_{23} + E_{56}$	$(-1, 2)$
	$E_\beta = E_{12} + \sqrt{2}E_{34} + \sqrt{2}E_{45} + E_{67}$	$(1, -1)$
	$E_{\alpha+\beta} = -E_{13} + \sqrt{2}E_{24} - \sqrt{2}E_{46} + E_{57}$	$(0, 1)$
	$E_{\alpha+2\beta} = -\sqrt{2}E_{14} + E_{25} + E_{36} - \sqrt{2}E_{47}$	$(1, 0)$
	$E_{\alpha+3\beta} = -E_{15} + E_{37}$	$(2, -1)$
	$E_{2\alpha+3\beta} = E_{16} + E_{27}$	$(1, 1)$

We shall define the generators according to the following principles: (1) The generators of a subgroup must be linear combinations of those of the larger group. (2) The weight operators of a subgroup should be so chosen that the highest weight state of the largest irrep of the subgroup is also a highest weight state of the larger group. We shall explain this point later. (3) The generators

Table 3. The algebraic basis (generators) of $SO(3)$

$L_z = 3E_{11} + 2E_{22} + E_{33} - E_{55} - 2E_{66} - 3E_{77}$
$L_+ = \sqrt{10}(E_{23} + E_{56}) + \sqrt{6}(E_{12} + \sqrt{2}E_{34} + \sqrt{2}E_{45} + E_{67})$
$L_- = \sqrt{10}(E_{32} + E_{65}) + \sqrt{6}(E_{21} + \sqrt{2}E_{43} + \sqrt{2}E_{54} + E_{76})$

must satisfy the following Cartan–Weyl commutation relations:

$$[H_i, H_j] = 0, \qquad 1 \leqslant i, j \leqslant i, \tag{8}$$

$$[H_i, E_\alpha] = \alpha_i E_\alpha, \tag{9}$$

$$[E_\alpha, E_{-\alpha}] = \sum \alpha^i H_i, \tag{10}$$

$$[E_\alpha, E_\beta] = N_{\alpha\beta} E_{\alpha+\beta}. \tag{11}$$

The generators satisfying these requirements have been found. They are given in Table 1 ($SO(7)$), Table 2 (G_2) and Table 3 ($SO(3)$). In Tables 1 and 2 the eigenvalues α_i (defined in Eq. (8)) are written in parentheses after the corresponding roots. The negative operators are not given in the tables, but they may be easily obtained by replacing the raising generators by corresponding lowering generators. It is a good exercise to check lengths of roots, angles between two simple roots and so on for these groups, keeping in mind the following definition of the scalar product of two roots

$$(\alpha, \beta) = \sum_{i=1}^{l} a^i \beta_i. \tag{12}$$

It should be noted that when the check is done for G_2, E_α, $E_{\alpha+3\beta}$ and $E_{2\alpha+3\beta}$ should be multiplied by $\sqrt{(3/2)}$ and E_β, $E_{\alpha+\beta}$ and $E_{\alpha+2\beta}$ by $\sqrt{(1/2)}$ to obtain true values of lengths and angles.

It should be noticed that there may be other choices of the generators. For example, it can be verified that $H'_1 = E_{11} + E_{22} - E_{66} - E_{77}$ and $H'_2 = -E_{22} + E_{33} - E_{55} + E_{66}$ are equivalent to ours in the sense that the same highest weight states are produced, but the labellings will be different. Sviridov et al. [19] and Parantonopoulos [20] defined generators of G_2 different from ours. In the work of Sviridov et al., the weight operators were defined $H'_1 = E_{11} + E_{22} - E_{66} - E_{77}$ and $H'_2 = E_{11} - E_{22} + 2E_{33} - 2E_{55} + E_{66} - E_{77}$. Parantopoulos's generators are then not Cartan–Weyl basis.

4. Irreps and weight sets of $SO(7)$ and G_2

In the algebraic representation theory of Lie groups, a basis function is usually associated with a definite wieght, i.e. the eigenvalue set of the weight operators H_i $(i = 1, \ldots, l)$. The highest weight will be used to label the irrep. In this paper we label irreps of $SO(7)$ with $W=(w_1, w_2, w_3)$ and the irreps of G_2 with $U=(u_1, u_2)$. For $SO(7)$, suppose that $|\Lambda_0\rangle$ is the function of the highest weight, then

$$H_i|\Lambda_0\rangle = w_i|\Lambda_0\rangle, \qquad i=1,\ 2 \text{ and } 3, \tag{13}$$

with the weight operators defined in the last section, and W the standard labelling adopted by Racah [1].

The weights can also be expressed as linear combinations of simple roots. Thus we may write the weights of $SO(7)$ as $\sum k_j\alpha_j$ and those of G_2 as $k_\alpha\alpha + k_\beta\beta$; these will be used to label rows or states of an irrep. If we denote the highest weight of an irrep of $SO(7)$ as $\sum k_{j0}\alpha_j$, then k_{j0} correlate to w_i by the following equations [16]:

$$\sum_{j=1}^{3} k_{j0}\frac{2(\alpha_j, \alpha_i)}{(\alpha_i, \alpha_i)} = w_i - w_{i+1} \qquad (i=1,2), \tag{14}$$

$$\sum_{j=1}^{3} k_{j0}\frac{2(\alpha_j, \alpha_3)}{(\alpha_3, \alpha_3)} = 2w_3. \tag{15}$$

Similarly if we denote the highest weight of an irrep of G_2 as $k_0\alpha + k_0\beta$, then $(k_{\alpha 0}, k_{\beta 0})$ can be calculated from the following set of equations:

$$-k_{\alpha 0} + k_{\beta 0} = u_1, \tag{16}$$

$$2k_{\alpha 0} - k_{\beta 0} = u_2. \tag{17}$$

In Figs. 1 and 2 the relation between the two symbols is useful to decide the irreps of G_2 or $SO(3)$.

Now let us determine the weight sets of irreps of $SO(7)$ and G_2. This is a simple task for low-dimensional irreps since the weight sets of $SO(7)$ and G_2 irreps of dimensions smaller than 100 have been published in appendix 1 in Cornwell's book [21]. For irreps of larger dimensions, their weights and corresponding multiplicities can be obtained by decomposing the Kronecker products of irreps of lower dimensions. In Tables 4 and 5, all the necessary decomposition formulas are displayed. It is easily seen from Table 4 that three weight sets must be known to work out the weights and their multiplicities appearing in

Table 4. Kronecker products of $SO(7)$ irreps

$(100)\times(100)=(000)+(110)+(200)$
$(100)\times(110)=(100)+(111)+(210)$
$(100)\times(111)=(110)+(111)+(211)$
$(110)\times(110)=(000)+(110)+(111)+(211)+(200)+(220)$
$(110)\times(111)=(100)+(110)+(111)+(210)+(211)+(221)$
$(111)\times(111)=(000)+(100)+(110)+(111)+(200)+(210)$ $+(211)+(220)+(221)+(222)$

Table 5. Kronecker products of G_2 irreps

$(10) \times (10) = (00) + (10) + (11) + (20)$
$(10) \times (11) = (10) + (20) + (21)$
$(10) \times (20) = (10) + (11) + (20) + (21) + (30)$
$(11) \times (11) = (00) + (11) + (20) + (30) + (22)$
$(11) \times (20) = (10) + (11) + (20) + (21) + (30) + (31)$
$(20) \times (20) = (00) + (10) + (11) + 2(20) + 2(21) + (30) + (22) + (31) + (40)$

the f-shell problems. They are

$$(100)\colon\ 0,\ \pm\alpha_3,\ \pm(\alpha_2+\alpha_3),\ \pm(\alpha_1+\alpha_2+\alpha_3).$$

$$(110)\colon\ 0^{(3)},\ \pm\alpha_1,\ \pm\alpha_2,\ \pm\alpha_3,\ \pm(\alpha_1+\alpha_2),\ \pm(\alpha_2+\alpha_3),\ \pm(\alpha_1+\alpha_2+\alpha_3)$$
$$\pm(\alpha_2+2\alpha_3),\ \pm(\alpha_1+\alpha_2+2\alpha_3),\ \pm(\alpha_1+2\alpha_2+2\alpha_3).$$

$$(111)\colon\ 0^{(3)},\ \pm\alpha_1,\ \pm\alpha_2,\ \pm\alpha_3^{(2)},\ \pm(\alpha_1+\alpha_2),\ \pm(\alpha_1+\alpha_3),\ \pm(\alpha_1-\alpha_3),$$
$$\pm(\alpha_2+\alpha_3)^{(2)},\ (\alpha_2+2\alpha_3),\ \pm(\alpha_1+\alpha_2+\alpha_3)^{(2)},\ \pm(\alpha_1+2\alpha_2+\alpha_3),$$
$$\pm(\alpha_1+\alpha_2+2\alpha_3),\ \pm(\alpha_1+2\alpha_2+2\alpha_3),\ \pm(\alpha_1+2\alpha_2+3\alpha_3),$$

where the superscripts in some weights are their multiplicities. The weight set of the irrep (110) is shown in Fig. 1. In this figure a weight $(k_1\alpha_1+k_2\alpha_2+k_3\alpha_3)$ is simply represented by $(k_1k_2k_3)$. Three possible ways of lowering a weight are represented by three lines of different slopes. Weights have been graded according to their values of $\sum k_j$. Weights having the same value of $\sum k_j$ are located in a horizontal level. The vertical line on the left side of the figure has been marked with the weights of G_2 corresponding to those of $SO(7)$ when the weights are the highest.

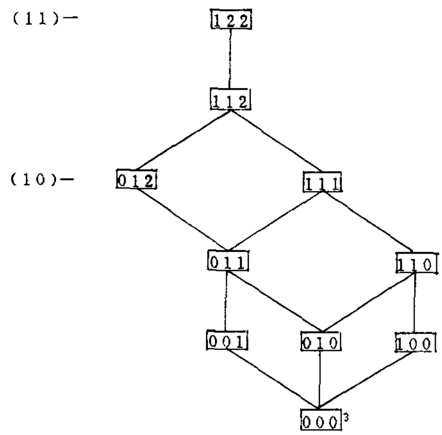

Fig. 1. The weight set of (110)

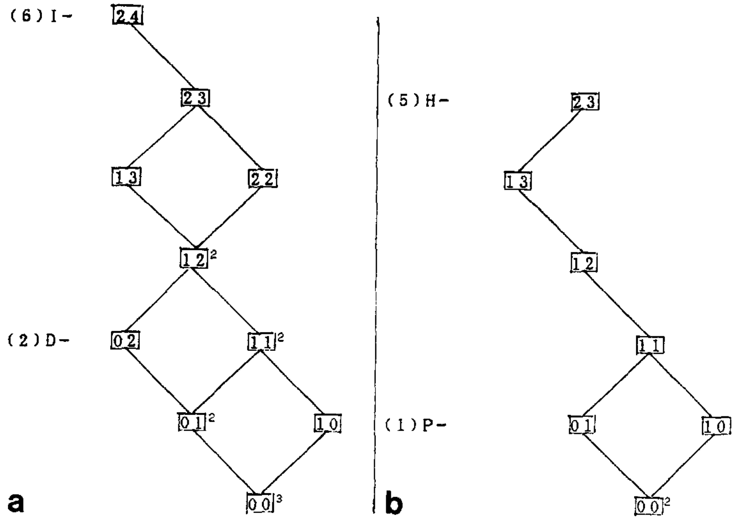

Fig. 2. Weight sets for G_2. (**a**) The weight set of (20); (**b**) the weight set of (11)

For G_2, only two weight sets are needed. They are

$$(10)\colon\ 0,\ \pm\beta,\ \pm(\alpha+\beta),\ \pm(\alpha+2\beta),$$

$$(11)\colon\ 0^{(2)},\ \pm\alpha,\ \pm\beta,\ \pm(\alpha+\beta),\ \pm(\alpha+2\beta),\ \pm(\alpha+3\beta),\ \pm(2\alpha+3\beta).$$

As an example, let us work out the weight set of (20). The weight set of the Kronecker product $(10)\times(10)$ is

$$0^{(7)},\ \pm\alpha^{(2)},\ \pm\beta^{(4)},\ \pm 2\beta,\ \pm(\alpha+\beta)^{(4)},\ \pm(\alpha+2\beta)^{(4)},\ \pm(\alpha+3\beta)^{(2)},$$
$$\pm(2\alpha+2\beta),\ \pm(2\alpha+3\beta)^{(2)},\ \pm(2\alpha+4\beta).$$

From this weight set we may obtain that of the irrep (20) by subtracting the weight sets of the irreps (00), (10) and (11)

$$(20)\colon\ 0^{(3)},\ \pm\alpha,\ \pm\beta^{(2)},\ \pm 2\beta,\ \pm(\alpha+\beta)^{(2)},\ \pm(\alpha+2\beta)^{(2)},\ \pm(\alpha+3\beta),$$
$$\pm(2\alpha+2\beta),\ \pm(2\alpha+3\beta),\ \pm(2\alpha+4\beta).$$

The weight sets of (20) and (11) are shown in Fig. 2. This figure is similar in meaning to Fig. 1. Here there are only two possible ways of lowering a weight for G_2. On the left of the figure the terms included in (20) are indicated.

5. Symmetry adapted functions

The functions adapted to group chain (1) are labelled as $|WU, \xi^{2s+1}LM_L\rangle$, where W and U stand for $SO(7)$ and G_2 irreps, S, L and M_L have their common meanings, and the additional index ξ identifies irreps repeatedly appearing in $G_2 \supset SO(3)$. If the adaptation to a finite group is considered, $\Gamma\gamma$ will be introduced into the state labelling to indicate its irrep and row. Symmetry adapted functions will be constructed in sequence along the group chain (1). For constructing symmetry functions adapted in every continuous group we need to know

(i) the algebraic basis in terms of $U(7)$ generators,
(ii) the weight sets of the group,
(iii) the highest weight functions corresponding to a given irrep.

Answers to (i) and (ii) have been given in the previous sections. We now consider how to establish the highest weight functions. If an irrep of $SO(7)$ or G_2 is the largest component in the reduction $U(7) \supset SO(7)$ or $U(7) \supset G_2$, the highest weight function belonging to the largest component is easily obtained. The largest component here means the irrep of the highest weight presented in reductions of irrep of $U(7)$ to that of $SO(7)$. For the largest component, the highest weight function of the subgroup is identical with that of the large group. If the large group is $U(7)$, the highest weight function consists of only one Gelfand state. For example $|(3110000)\rangle$ is the highest Gelfand state of [211] of $U(7)$, it is therefore the highest weight function for (211) of $SO(7)$ and also the highest one for (30) of G_2. This can be verified by using the weight operators of these groups and Eq. (19). In order to establish the highest weight functions in a general case, the first step is to find Gelfand states of the given weight, and write the function as

$$|\Lambda_0\rangle = \sum_i C_i |(d_r)_i\rangle. \tag{18}$$

Then the coefficients C_i are determined from the highest weight condition,

$$E_{\alpha_i}|\Lambda_0\rangle = 0, \qquad \alpha_i > 0. \tag{19}$$

The lowest weight function can be similarly established.

Asherova and Smirnov [22] proposed a very general method of finding the highest weight functions for a compact group. They defined the projection operator,

$$P^{[\lambda]} = \prod_{\alpha > 0} P_\alpha^{[\lambda]}, \tag{20}$$

where $[\lambda]$ was the highest weight and the operator $P_\alpha^{[\lambda]}$ was defined as

$$P_\alpha^{[\lambda]} = \sum_{t=0}^{\infty} (-t)^t \frac{2^t \left[\dfrac{2(\alpha, \Lambda + g)}{(\alpha, \alpha)}\right]^{1/2}}{(\alpha, \alpha)^t t! \left[\dfrac{2(\alpha, \Lambda + g)}{(\alpha, \alpha)} + t\right]!} E_{-\alpha}^t E_\alpha^t \tag{21}$$

with

$$g = 1/2 \sum_{\alpha > 0} \alpha. \tag{22}$$

Although this method has some advantages we find that is it not convenient for our purposes.

Knowing the highest weight function $|\Lambda_0> = \sum k_{i0}\alpha_i$ or the lowest weight function $|-\Lambda_0\rangle = -\sum k_{i0}\alpha_i$, we can construct functions of an arbitrary weight $\sum k_i\alpha_i$ from the following formulas:

$$\left|\sum_i k_i\alpha_i\right\rangle = CE_{-\alpha_1}^{\Delta k_1} E_{-\alpha_2}^{\Delta k_2} \cdots E_{-\alpha_i}^{\Delta k_i}|\Lambda_0\rangle, \tag{23}$$

or

$$\left|\sum_i k_i\alpha_i\right\rangle = C'E_{\alpha_1}^{\Delta k_1'} E_{\alpha_2}^{\Delta k_2'} \cdots E_{\alpha_i}^{\Delta k_i'}|-\Lambda_0\rangle, \tag{24}$$

where E_{α_i} and $E_{-\alpha_i}$ are raising and lowering operators, respectively. C and C' are normalization coefficients, and

$$\Delta k_i = k_{i0} - k_i \tag{25}$$

and

$$\Delta k_i' = k_{i0} + k_i. \tag{26}$$

If a weight is non-degenerative, only one function is obtained. If it is degenerate several independent, but not necessarily orthogonal, functions, can be obtained. In the latter case the functions may be orthogonalized.

Let us now construct the symmetry functions associated with the irrep (110) of $SO(7)$ and with some irreps of its subgroups. Suppose (110) comes from the reduction of the irrep [211] of $U(7)$. Of the 210 Gelfand states of [211], 6 have the weight (110). Taking a linear combination of the 6 states and acting on the combination with the raising operators cited in Table 1, we obtain a set of equations for the coefficients. Solving them gives the highest weight function (here the labellings [211] and (110) have been dropped)

$$\begin{aligned}|(\alpha_1+2\alpha_2+2\alpha_3)\rangle = 1/\sqrt{5}[|(3100001)\rangle - |(1300010)\rangle \\ + 2/\sqrt{3}|(1100200)\rangle + \sqrt{6}/3|(1120100)\rangle - |(1103000)\rangle].\end{aligned} \tag{27}$$

The other weight functions belonging to (110) can be found from $|(\alpha_1+2\alpha_2+2\alpha_3)\rangle$ by means of the lowering operators. For example,

$$\begin{aligned}|(\alpha_1+\alpha_2+2\alpha_3)\rangle &= E_{-\alpha_2}|(\alpha_1+2\alpha_2+2\alpha_3)\rangle \\ &= 1/\sqrt{5}[|3010001\rangle + 2\sqrt{3}/3|1110020 + \sqrt{6}/6|1120010\rangle \\ &\quad - \sqrt{2}/2|1210010\rangle + |1030100\rangle - |1013000\rangle].\end{aligned} \tag{28}$$

The procedure is continued until all the 21 functions of the irrep (110) are obtained. The results (only positive weight functions) are given in Table 6, where the three functions of weight 0 are defined as

$$|0(1)\rangle = 1/\sqrt{2}E_{-\alpha_1}|\alpha_1\rangle \tag{29}$$

$$|0(2)\rangle = 1/\sqrt{3}[1/\sqrt{2}E_{-\alpha_1}|\alpha_1\rangle - \sqrt{2}E_{-\alpha_2}|\alpha_2\rangle] \tag{30}$$

$$|0(3)\rangle = \sqrt{2}/\sqrt{3}[1/\sqrt{2}E_{-\alpha_1}|\alpha_1\rangle - \sqrt{2}E_{-\alpha_2}|\alpha_2\rangle] + \sqrt{3}E_{-\alpha_3}|\alpha_3\rangle. \tag{31}$$

Table 6. The basis functions of (110)

$|(\alpha_1+2\alpha_2+2\alpha_3)\rangle = 1/\sqrt{5}[|3100001\rangle - |1300010\rangle + 2/\sqrt{3}|1110200\rangle + \sqrt{6}/3|1120110\rangle - |1103000\rangle]$
$|(\alpha_1+\alpha_2+2\alpha_3)\rangle = 1/\sqrt{5}[|3010001\rangle + 2\sqrt{3}/3|1110020\rangle - \sqrt{6}/6|1120010\rangle - \sqrt{2}/2|1210010\rangle + |1030100\rangle - |1013000\rangle]$
$|(\alpha_1+\alpha_2+\alpha_3)\rangle = 1/\sqrt{5}[|3001001\rangle + 2\sqrt{3}/3|1101020\rangle - \sqrt{6}/6|1102010\rangle - \sqrt{2}/2|1201010\rangle - 2\sqrt{3}/3|1011200\rangle + \sqrt{6}/6|1012100\rangle + \sqrt{2}/2|1021100\rangle]$
$|(\alpha_2+2\alpha_3)\rangle = 1/\sqrt{5}[2\sqrt{3}/3|1110002\rangle - \sqrt{6}/6|1120001\rangle + \sqrt{2}/2|1210001\rangle - |0310010\rangle + |0130100\rangle - |0113000\rangle]$
$|(\alpha_2+\alpha_3)\rangle = 1/\sqrt{10}[2\sqrt{6}/3|1101002\rangle + \sqrt{3}/3|1102001\rangle + |1201001\rangle - \sqrt{2}|0301010\rangle - 2\sqrt{6}/3|0111200\rangle + \sqrt{3}/3|0112100\rangle + |0121100\rangle]$
$|(\alpha_1+\alpha_2) = 1/\sqrt{5}[|3000101\rangle + 2\sqrt{3}/3|1100120\rangle - \sqrt{6}/6|1100210\rangle - \sqrt{2}/2|1200110\rangle - |1010300\rangle + |1003100\rangle]$
$|\alpha_1\rangle = 1/\sqrt{5}[|3000011\rangle + |1100030\rangle - \sqrt{6}/2|1010210\rangle - \sqrt{2}/2|1020110\rangle + |1003010\rangle]$
$|\alpha_2\rangle = 1/\sqrt{5}[2\sqrt{3}/3|1100102\rangle - \sqrt{6}/6|1100201\rangle + \sqrt{2}+2|1200101\rangle - |0300110\rangle - |0110300\rangle + |0103100\rangle]$
$|\alpha_3\rangle = 1/\sqrt{10}[2\sqrt{6}/3|1011002\rangle - \sqrt{3}/3|1012001\rangle + 1021001\rangle - 2\sqrt{6}/3|0111020\rangle + \sqrt{3}/3|0112010\rangle - |0121010\rangle + \sqrt{2}|0031100\rangle]$
$|0(1)\rangle = 1/\sqrt{60}[2\sqrt{2}|1100012\rangle + 2|1100021\rangle + 2\sqrt{3}|1200011\rangle - 3|1010201\rangle - \sqrt{3}|1020101\rangle + \sqrt{6}|1003001\rangle - 3|0110210\rangle - \sqrt{3}|0120110\rangle + \sqrt{6}|0103010\rangle]$
$|0(2)\rangle = 1/\sqrt{60}[-2\sqrt{2}/\sqrt{3}|1100012\rangle - 4\sqrt{2}/\sqrt{3}|1010102\rangle + 4\sqrt{3}|1100021\rangle - \sqrt{12}/6|1010201\rangle - 3|1020101\rangle + \sqrt{2}|1003001\rangle + 4\sqrt{2}/\sqrt{3}|0110120\rangle + \sqrt{12}/6|0110210\rangle + 3|0120110\rangle - \sqrt{2}|0103010\rangle - 2\sqrt{2}|0013100\rangle]$
$|0(3)\rangle = 1/\sqrt{60}[-4\sqrt{3}/3|1100012\rangle + 4\sqrt{3}/3|1010102\rangle + 4\sqrt{6}/3|1100021\rangle - 4\sqrt{6}/3|1010201\rangle + 2|1003001\rangle - 4\sqrt{3}/3|0110120\rangle + 4\sqrt{6}/3|0110210\rangle - 2|0103010\rangle + 2|0013100\rangle]$

Under the reduction $SO(7) \supset G_2$, (110) is decomposed into (11) and (10). The highest weight function of (11) is the same as that of (110), i.e.

$$|(11)(2\alpha+3\beta)\rangle = |(\alpha_1+2\alpha_2+2\alpha_3)\rangle. \tag{32}$$

Starting from function (32), basis functions belonging to (11) can be obtained by applying the lowering operators of G_2 to function (29). This procedure is considerably simplified by the relation between operators of G_2 and those of $SO(7)$. For example,

$$\begin{aligned} |(11)(\alpha+2\beta)\rangle &= E_{-\beta}|(11)(\alpha+3\beta)\rangle \\ &= (E_{-\alpha_1}+\sqrt{2}E_{-\alpha_3})|(\alpha_1+\alpha_2+2\alpha_3)\rangle \\ &= 1/\sqrt{3}[|(\alpha_2+2\alpha_3)\rangle + \sqrt{2}|(\alpha_1+\alpha_2+\alpha_3)\rangle]. \end{aligned} \tag{33}$$

Table 7. The transformation coefficients of $SO(7) \supset G_2$ reduction

$SO(7)$	G_2											
	(11)								(10)			
	$2\alpha+3\beta$	$\alpha+3\beta$	$\alpha+2\beta$	$\alpha+\beta$	α	β	$O(1)$	$O(2)$	$\alpha+2\beta$	$\alpha+\beta$	β	0
(110)												
$\alpha_1+2\alpha_2+2\alpha_3$	1											
$\alpha_1+\alpha_2+2\alpha_3$		1										
$\alpha_1+\alpha_2+\alpha_3$			$\sqrt{6}/3$						$\sqrt{3}/3$			
$\alpha_2+2\alpha_3$			$\sqrt{3}/3$						$-\sqrt{6}/3$			
$\alpha_1+\alpha_2$				$\sqrt{3}/3$						$\sqrt{6}/3$		
$\alpha_2+\alpha_3$				$\sqrt{6}/3$						$-\sqrt{3}/3$		
α_1						$\sqrt{3}/3$					$\sqrt{6}/3$	
α_2					1							
α_3						$\sqrt{6}/3$					$-\sqrt{3}/3$	
$O(1)$							1/2	$\sqrt{3}/6$				$\sqrt{6}/3$
$O(2)$							$-\sqrt{3}/2$	1/6				$\sqrt{2}/3$
$O(3)$								$\sqrt{8}/3$				$-1/3$

The other functions can be similarly established. They are given in Table 7. The two functions of weight 0 have been orthogonalized and have the forms

$$|(11)0(1)\rangle = 1/\sqrt{2}E_{-\alpha}|\alpha\rangle, \tag{34}$$

$$|(11)0(2)\rangle = \sqrt{3}[1/\sqrt{2}E_{-\alpha}|\alpha\rangle - \sqrt{6}/3E_{-\beta}|\beta\rangle]. \tag{35}$$

The highest weight expressed in simple roots for the component (10) of G_2 is also equal to $(\alpha + 2\beta)$. We have found that the function corresponding this weight is

$$|(10)(\alpha + 2\beta)\rangle = 1/\sqrt{3}[|(\alpha_1 + \alpha_2 + \alpha_3)\rangle - \sqrt{2}|(\alpha_2 + 2\alpha_3)\rangle]. \tag{36}$$

It is obviously orthogonal to $|(11)(\alpha + 2\beta)\rangle$. This is the first member of the function set spanning the irrep (10) of G_2. The other members are given in Table 7.

We now consider the reduction of G_2 to $SO(3)$. L_z can be written as

$$L_z = 3H_1 + 2H_2, \tag{37}$$

where H_1 and H_2 are weight operators of G_2. This form reminds us that L_z is diagonal in the G_2, $SO(7)$ and $U(7)$ bases. This result comes, in fact, from our choice of the one-electron orbitals. Applying L_z to the function set of (11), we obtain the following diagonal matrix elements (see Fig. 2):

$$[5, 4, 3, 2, 1, 1, 0, 0, -1, -1, -2, -3, -4, -5].$$

This indicates that the terms ^3H and ^3P are included in the decomposition of (11) in accord with the branch rule. The function of $M_L = 5$ is equal to $|(11)(2\alpha + 3\beta)\rangle$, which is the starting point for finding all ^3H symmetry functions. The functions, together with those of ^3P and ^3F (coming from (10) of G_2), are given in Table 8.

Table 8. The transformation coefficients of $G_2 \supset SO(3)$ reduction

G_2	$SO(3)$											
	H						P		F			
	5	4	3	2	1	0	1	0	3	2	1	0
(11)												
$2\alpha + 3\beta$	1											
$\alpha + 3\beta$		1										
$\alpha + 2\beta$			1									
$\alpha + \beta$				1								
α					$3/\sqrt{14}$		$\sqrt{5}/\sqrt{14}$					
β					$\sqrt{5}/\sqrt{14}$		$-3/\sqrt{14}$					
0(1)						$\sqrt{27}/\sqrt{28}$		$1/\sqrt{28}$				
0(2)						$-1/\sqrt{28}$		$\sqrt{27}/\sqrt{28}$				
(10)												
$\alpha + 2\beta$									1			
$\alpha + \beta$										1		
β											1	
0												1

Finally let us say a few words about the adaptation to a finite group. Kent and Schlesinger [23] suggested the method of projection operators for producing symmetry adapted functions of a finite group. We find that their projection operators are too complicated when the number of electrons is large. We would rather make use of the subduction coefficients for $SO(3) \supset G$ [24]. For example from the subduction coefficients of $SO(3) \supset 0$ and from Tables 6–8 we can write down the symmetry functions of a T_2 species in an octahedral field.

$$\begin{aligned}|[211](110)(11)^3HT_20\rangle = 1/6\sqrt{30}[&6|1010003\rangle + 4\sqrt{6}|1001012\rangle \\ &+ 4\sqrt{6}|1101002\rangle - 2\sqrt{3}|1001021\rangle - 3\sqrt{6}|0110021\rangle \\ &+ 6|1002011\rangle + 3\sqrt{2}|0120011\rangle - 6|0030101\rangle \\ &+ |3000101\rangle + 6|0013001\rangle + 2\sqrt{3}|1102001\rangle \\ &+ 6|1201001\rangle - 6\sqrt{2}|0101030\rangle + 4\sqrt{3}|1100120\rangle \\ &+ 6\sqrt{3}|0011210\rangle - \sqrt{6}|1100210\rangle - 6|0012110\rangle \\ &- 3\sqrt{2}|1200110\rangle - 6\sqrt{2}|0301010\rangle - 6|1010300\rangle \\ &- 4\sqrt{6}|0111200\rangle + 6|1003100\rangle + 2\sqrt{3}|0112100\rangle \\ &+ 6|0121100\rangle]\end{aligned} \tag{38}$$

$$\begin{aligned}|[211](110)(11)^3HT_21\rangle = 1/8\sqrt{15}[&3\sqrt{10}|1000013\rangle - \sqrt{10}|1100003\rangle \\ &- 6\sqrt{2}|1010012\rangle - 4\sqrt{5}/\sqrt{3}|1001102\rangle \\ &- 2\sqrt{2}|111002\rangle - 3\sqrt{10}|0100031\rangle + \sqrt{5}|0001121\rangle \\ &- 3\sqrt{10}|0010121\rangle + 3|1010021\rangle + 6\sqrt{5}|0010211\rangle \\ &- 3\sqrt{3}|1020011\rangle - \sqrt{10}|0300011\rangle \\ &- \sqrt{10}/\sqrt{3}|1001201\rangle + \sqrt{15}|0110201\rangle \\ &- \sqrt{10}|1002101\rangle - \sqrt{10}|0103001\rangle \\ &- 2\sqrt{3}|3001001\rangle + |1120001\rangle - \sqrt{3}|1210001\rangle \\ &+ 3\sqrt{6}|0110030\rangle + 4\sqrt{5}/\sqrt{3}|0101120\rangle - 4|1101020\rangle \\ &- \sqrt{10}/\sqrt{3}|0101210\rangle + \sqrt{10}|0102110\rangle \\ &+ 3\sqrt{6}|0030110\rangle - 3\sqrt{6}|0013010\rangle + \sqrt{2}|1102010\rangle \\ &+ \sqrt{6}|1201010\rangle + \sqrt{6}|0310010\rangle - \sqrt{20}|0011300\rangle \\ &+ 4|0111200\rangle - \sqrt{2}|1012100\rangle - \sqrt{6}|1021100\rangle \\ &- \sqrt{6}|0130100\rangle + \sqrt{6}|0113000\rangle],\end{aligned} \tag{39}$$

$$
\begin{aligned}
|[211](110)(11)^3HT_2-1\rangle = 1/8\sqrt{15}[&-2\sqrt{3}|1001003\rangle-2\sqrt{2}|1000112\rangle\\
&-6\sqrt{2}|1100102\rangle-4\sqrt{5}/\sqrt{3}|1011002\rangle\\
&+|1000121\rangle+3\sqrt{2}|0101021\rangle-\sqrt{3}|1000211\rangle\\
&-\sqrt{6}|0102011\rangle-\sqrt{10}|3000011\rangle-3\sqrt{2}|0011201\rangle\\
&+3|1100201\rangle+\sqrt{6}|0012101\rangle-3\sqrt{3}|1200101\rangle\\
&+\sqrt{10}/\sqrt{3}|1012001\rangle-\sqrt{10}|1021001\rangle\\
&+3\sqrt{10}|3100001\rangle-\sqrt{6}|0100130\rangle\\
&-\sqrt{10}|1100030\rangle+4\sqrt{5}/\sqrt{3}|0111020\rangle\\
&-\sqrt{6}|0010310\rangle+\sqrt{15}|1010210\rangle+\sqrt{6}|0003110\rangle\\
&+\sqrt{5}|1020110\rangle+3\sqrt{6}|0300110\rangle-\sqrt{10}|1003010\rangle\\
&-\sqrt{10}/\sqrt{3}|0112010\rangle-\sqrt{10}|0121010\rangle\\
&-3\sqrt{10}|1300010\rangle+3\sqrt{6}|0110300\rangle\\
&+2\sqrt{30}|1110200\rangle-3\sqrt{6}|0103100\rangle\\
&-\sqrt{20}|0031100\rangle+2\sqrt{15}|1120100\rangle\\
&-3\sqrt{10}|1103000\rangle]. \qquad (40)
\end{aligned}
$$

6. Discussion

Constructing symmetry functions adapted to a given group chain is an interesting and active subject. In this paper the functions adapted to group chain (1) have been constructed by the Lie algebra technique and expanded in terms of the Gelfand basis. In this approach, except for the trivial cases, the most troublesome step is finding the highest weight states. As a result in order to determine the coefficients in Eq. (18), a set of equations (19) must be solved. If the symmetry adaptation to $SO(7)$ and G_2 is not considered, there will be more coefficients, and in addition the number of equations provided only by the highest weight condition $L_+|LL\rangle=0$ is insufficient to determine the coefficients. Zhang suggested [25] that this set of equations can be augmented if the state is chosen to be an eigenvector of the Casimir operations of $SO(7)$ and G_2. The number of the coefficients does not decrease. For the example mentioned in the introduction the 58 coefficients in the linear combination of the Gelfand states need to be determined to find 10 states of $|^2F3\rangle$. The highest weight conditions can only provide 48 equations. The Casimir operators and normalization gives 9 of the additional 10 needed equations. The fact that one equation is missing is associated with the fact that there are two functions of $|[2221](221)(31)^2F3\rangle$. The same feature exists in our approach, though the number of the coefficients to be determined is only 13.

The state $|LL\rangle$ can be found by a projection operator, say the Lowdin operator [26],

$$P^L = \prod_{K \neq L} \frac{\hat{L}_- \hat{L}_+ + \hat{L}_Z^2 + \hat{L}_Z - K(K+1)}{L(L+1) - K(K+1)}. \tag{41}$$

This method is convenient only when the values of K are known. Extra quantum number must also be assigned to the states of the same L.

Our approach has an additional advantage that it allows us to calculate the subduction coefficients of $U(7) \supset SO(7)$, $SO(7) \supset G_2$ and $G_2 \supset SO(3)$. In order to do this a little more effort is required to orthogonalize the states of the same weight which is not needed if we are only interested in finding the term functions. The values given in Tables 6–8 are, in fact, the subduction coefficients. Once the subduction coefficients have been found, we may construct the generator matrices and furthermore calculate the CG coefficients of $SO(7)$ and G_2. We shall discuss these problems in future applications.

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