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The Computation of the Representation Matrices of the Generators of the Unitary Group*

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A method is presented for the efficient computation of the representation matrices of the unitary group, $U(n)$ in the Gelfand–Tsetlin basis (corresponding to the usual spin-symmetry adapted basis for an N electron CI). The present scheme is conceptually and computationally attractive in that it is formulated directly in terms of Weyl tableaux and also that it permits simultaneous basis vector generation and matrix element evaluation. In addition the basis vectors are ordered so that subsequent restriction to the three dimensional rotation group is facilitated. An illustrative example is also presented.

Key words: Representation matrices of the unitary group – Configuration interaction – symmetric group

1. Introduction

In the traditional approach to the method of configuration interaction (CI) the central theoretical and practical problems are associated with the efficient generation of the symbolic form of the one- and two particle density matrices (so called symbolic matrix elements). However, when the Hamiltonian is written in "second quantized form" it becomes a sum of linear and bilinear forms in the generators of the unitary group $U(n)$, where n is the member of single particle basis states (i.e. orbitals). Thus the problem of the computation of symbolic matrix elements reduces to one of evaluating matrix elements of the generators of $U(n)$ in the N-electron CI basis. The relationship between the unitary group method and traditional methods are reviewed in Paldus' paper [1]. We wish to emphasise, however, that the unitary group approach offers definite advantages, since once the linear (one-electron) part of the Hamiltonian is computed, the bilinear (two-

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electron) part may be computed by matrix multiplication (with highly structured very sparse matrices).

Paldus' approach [1–3] to the problem of the construction of the generators of $U(n)$ is essentially a simplification of the method of Gelfand and Tsetlin [4]. This simplification is possible because of the unnecessary generality of the Gelfand method when applied to electronic systems, and leads to enormous simplification of the generator matrix element formulae. Harter [5, 6] has also outlined a scheme, in which the generator matrix elements are calculated by a "jawbone" formula. His system has the conceptual advantage that it is easily interpreted in terms of the intuitively appealing Weyl tableaux but the disadvantage that the "jawbone" formulae are not suitable for automatic computation. However, Harter generates the basis vectors in the same way as Paldus using branching rules, so that Gelfand tableaux are generated and then converted to Weyl tableaux.

2. Basis Vectors for Irreducible Representations of $U(n)$

In the Gelfand–Tsetlin approach the basis vectors are obtained by a branching pattern in which all lexical tableaux are obtained from the one of the highest weight. The first row of the highest weight tableau (or any tableau obtained from it in the branching pattern) denotes the box structure of the Weyl tableau

$$m_n = [m_{1n}, m_{2n}, \ldots, m_{nn}] \tag{1}$$

where m_{kn} gives the number of boxes in the kth row of the usual Young diagram for S_N. Obviously, one has the relation

$$\sum_k m_{kn} = N \tag{2}$$

The basis vectors for $U(n)$ are now constructed by writing down all possible Gelfand tableaux

$$|m\rangle = \begin{bmatrix} m_{1n} \quad m_{2n} \quad \cdots\cdots\cdots\cdots \quad m_{nn} \\ m_{1,n-1} \quad m_{2,n-1} \quad m_{n-1,n-1} \\ \cdots\cdots \\ \cdots \\ m_{11} \end{bmatrix} \tag{3}$$

where one has the "betweenness condition"

$$m_{i,j+1} \geqslant m_{ij} \geqslant m_{i+1,j+1} \tag{4}$$

These conditions are simply restrictions on the branching diagrams for the subgroup chain

$$U(n) \supset U(n-1) \ldots U(1)$$

Each tableau which obeys these restrictions is referred to as a lexical tableau and if the restriction is applied leaving highest members in the highest rows first the tableaux are said to be in lexical order.

The Gelfand tableaux obtained in this manner are in one-to-one correspondence with Weyl tableaux. The number of boxes in the tableau is deduced from the number of non-zero entries in the top row of the Gelfand tableau. The numbers in the rows of the Weyl tableau are then given by the columns of the corresponding Gelfand tableau. In the kth row of the Weyl tableau the first m_{kk} entries correspond to the number of the row in which m_{kk} occurs. The following $m_{k,k+l}$-m_{kk} entries correspond to the row number in which $m_{k,k+l}$ occurs.

With a view to later discussion it should be pointed out that the *number i* contained in a Weyl tableau is related to row i of the corresponding Gelfand tableau. Thus a change in the i'th row of a Gelfand tableau corresponds to simply to the addition or removal of the number i from the Weyl tableau. In particular, we shall be concerned with the case when only the i'th row of the Gelfand tableau is allowed to change so that a given element in the row is increased from 0 to 1 or 1 to 2. This change implies that the number $i+1$ in the Weyl tableau is replaced by i in exactly the same position.

3. Matrix Elements of the Generators of $U(n)$

The infinitesimal generators of $U(n)$, E_{pq} obey the commutation relation (7)

$$[E_{pq}, E_{rs}] = \delta_{qr} E_{ps} - \delta_{ps} E_{rq} \tag{5a}$$

which reduces to

$$[E_{pr}, E_{rs}] = E_{ps} \tag{5b}$$

in the special case that $q=r$. The generators are divided into three types according to whether $p=q$, $p>q$ or $p<q$ corresponding to weight generators lowering generators and raising generators respectively. Since the E_{pq} are generators of $U(n)$ one also has the Hermitian conjugate condition

$$E_{pq}^{\dagger} = E_{qp} \tag{5c}$$

Since the matrix representations of the generators in the Gelfand basis have only real entries Eq. (5c) implies that the matrix representation of the operator E_{pq} is simply the transpose of that for E_{qp}. Also, because of the relationship (5b) it will be possible to calculate all the raising generators from a set of elementary raising generators E_{ij} where $j=i+1$. Thus, we are concerned only with the computation of the generators E_{ij} ($j=i+1$). The relationship of the generator matrix representations to the second quantized form of the Hamiltonian is outlined by Paldus [3]. The significant point to be made with a view to practical computation is that the Hamiltonian is a bilinear form in the generators and hence the eventual computation of the matrix representative of the Hamiltonian involves merely matrix multiplication of pairs of generator matrices.

Gelfand has given a general formula (4) for the computation of the matrix elements of the generators, which although quite general, is somewhat unwieldy. Paldus [1–3] has observed that for atomic and molecular applications Gelfand's formula is unnecessarily general since the entries in the Gelfand tableaux can take only values of 2, 1 or 0. Because of this Paldus has shown that one may contract the Gelfand tableaux in $3 \times n$ tableaux

$$m=\begin{bmatrix} m_{1n} & m_{2n} & \cdots\cdots & m_{nn} \\ & m_{1,n-1} & m_{2,n-1} & \cdots \\ & & m_{12} \quad m_{22} & \\ & & m_{11} & \end{bmatrix}=\begin{bmatrix} a_n & b_n & c_n \\ a_{n-1} & b_{n-1} & c_{n-1} \\ a_2 & b_2 & c_2 \\ a_1 & b_1 & c_1 \end{bmatrix} \tag{6}$$

which we shall refer to as Paldus tableaux. The entries in the Paldus tableaux are defined so that the numbers in the first column (a_l) correspond to the number of 2's in the l'th row of the equivalent Gelfand tableau, the numbers in the second column (b_l) to the ones in the l'th row and the numbers in the third column (c_l) to the o's in the l'th row.

The simplified matrix element formulae now follow directly. If there is to be a matrix element between an elementary raising operator E_{ij} $(j=i+1)$ between two basis states $|m\rangle$ and $|m'\rangle$, $\langle m|E_{ij}|m'\rangle$ then $|m'\rangle$ must differ by one from $|m\rangle$ in the i'th row of the Gelfand tableau. For electrons this implies that 0 or a 1 on the i'th row of $|m'\rangle$ is replaced by a 1 or a 2 respectively on the i'th row of $|m\rangle$ (any other change in the i'th row of the Gelfand tableau leads to a tableau that violates the betweenness conditions [3]). The simplified matrix element formula of Paldus can be separated for each of the two possibilities. The first situation which Paldus calls the type A relation arises when a 1 on the i'th row of $|m'\rangle$ is replaced by a 2 on the row of $|m\rangle$. In terms of the Paldus tableau a_i of $|m'\rangle$ is replaced by a_i+1 in $|m\rangle$, and b_i of $|m'\rangle$ is replaced by b_i-1 in $|m\rangle$. The simplified formula in this case is

$$\langle m|E_{ij}|m'\rangle=\left(\frac{b_i(b_i+1)}{(b_{i+1}+1)(b_{i-1}+1)}\right)^{1/2} \tag{7a}$$

The second possibility, type B arises when a 0 on the i'th row of $|m'\rangle$ is replaced by a 1 on the i'th row of $|m\rangle$ and thus b_i in $|m'\rangle$ is replaced by b_i+1 in $|m\rangle$ and c_i in $|m'\rangle$ is replaced by c_i-1 in $|m\rangle$ in the corresponding Paldus tableau. The formula in this case is

$$\langle m|E_{ij}|m'\rangle=\left(\frac{(b_i+1)(b_i+2)}{(b_{i+1}+1)(b_{i-1}+1)}\right)^{1/2} \tag{7b}$$

4. Matrix Element Formulae in Terms of Weyl Tableaux

The possible conditions for matrix elements just discussed can now be reinterpreted in terms of Weyl tableaux. As we shall presently discuss this leads to further simplification. We need, however, a compact method for writing a general Weyl tableau for an N electron situation. Thus, for a Weyl tableau as shown in Fig. 1 we define a line tableau

$$|m\rangle=|x_1, x_2, x_3 \ldots, x_t; y_1, y_2 \ldots, y_u\rangle \tag{8a}$$

which consists of the numbers in the first column of the Weyl tableau followed by

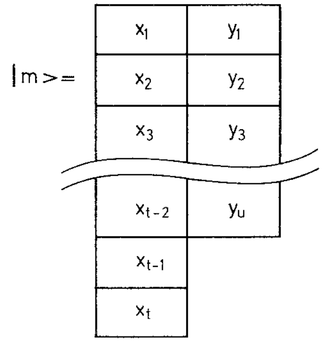

Fig. 1. A schematic representation of a Weyl tableau

the numbers in the second. Another different Weyl tableau may be distinguished by the line tableau

$$|m'\rangle = |x_1', x_2', \ldots, x_t'; y_1', y_2', \ldots, y_u'\rangle \tag{8b}$$

We can now distinguish the Paldus type A and B conditions using the Gelfand tableau/Weyl tableau relationship discussed in Sect. 2. The occurrence of the number $i+1(=j)$ in the Weyl tableau depends upon an increase in the entry in the j'th row over the i'th row of the Gelfand tableau. It follows that an increase in the i'th row can only change the number j to the number i in exactly the same position in the Weyl tableau. Thus, in the type A situation, where a 1 in the i'th row of $|m'\rangle$ is replaced by a 2 in the i'th row of $|m\rangle$, the change in the Weyl tableau must be to change j to i in the *same position* in the *second column*. This is so because the presence of a 2 above a 1 in a Gelfand column must introduce a number into the second column of the Weyl tableau. Thus in the notation of Eq. (8) the conditions for the existence of a matrix element of the generator E_{ij} $(j=i+1)$ between basis vectors $|m\rangle$ and $|m'\rangle$ are

$$\begin{aligned} &x_k = x_k' \quad \text{for all } k \\ &y_k = y_k' \quad \text{for all } k \text{ except where } y_k = i \text{ and } y_k' = j \text{ for } j = i+1 \end{aligned} \tag{9a}$$

Similarly for the type B situation where a 0 in the i'th row of the Gelfand tableau $|m'\rangle$ is replaced by a 1 in the i'th row of $|m\rangle$ the effect in the Weyl tableau is to change $j\,(=i+1)$ to i at the same position in the first column. Again, in the notation of Eq. (8) the matrix element condition for type B is

$$\begin{aligned} &y_k = y_k' \quad \text{for all } k \\ &x_k = x_k' \quad \text{for all } k \text{ except where } x_k = i \text{ and } x_k' = j \text{ for } j = i+1 \end{aligned} \tag{9b}$$

The type A and B cases might equally well be called the column 2 and column 1 cases when formulated in terms of Weyl tableaux.

The conditions for the existence of a matrix element of an elementary generator E_{ij}, $j=i+1$ between two basis vectors $|m\rangle$ and $|m'\rangle$ expressed as a line tableau may now be expressed very simply. All numbers in the two line tableaux $|m\rangle$ and $|m'\rangle$ must be the same except one which must have a j in $|m'\rangle$ replaced by i in $|m\rangle$

in exactly the same position. Having first identified a matrix element by this criteria it is a simple matter to identify it as A or B type by its position in the line tableau. It is not necessary in the present formulation to search for several pairs of basis vectors with a specific $i-j$ difference. Any pair $|m\rangle$ and $|m'\rangle$ related as in Eq. (9) will give rise to a matrix element of some elementary raising operator. Thus the elementary generator matrices need not be calculated in order. Indeed as we shall presently discuss, it is possible to evaluate the generator matrices as the basis vectors are generated.

In order to evaluate the matrix elements of the elementary generators using the Weyl tableau we must reinterpret the b_l of Eq. (7) in terms of the Weyl tableaux. The b_l correspond to the numbers of 1's on the l'th row of the Gelfand tableau. Now, using the relationship between Gelfand and Weyl tableaux, one can interpret b_l as the number of "unpaired" boxes (i.e. those for no y_k exists for a given x_k) in the Weyl tableau when boxes containing numbers greater than l have been removed from the tableau. This number is readily computed from the line tableau by counting the number of entries x_i up to and including x_l and subtracting from this the number of entries y_i up to and including y_l. Thus

$$b_l = \sum_{x_i} n_{x_i} - \sum_{y_i} n_{y_i} \tag{10}$$

where $n_{x_i}=1$ if $x_i \leqslant l$ and 0 otherwise and similarly for n_{y_i}. The three b_l values necessary for matrix element computation can be rapidly calculated in succession using Eq. (10).

The matrix elements of the weight generators E_{ii} are particularly easy to calculate in terms of Weyl tableau. The formula of Paldus is

$$\langle m|E_{ii}|m'\rangle = \delta_{mm'}[2(a_i - a_{i-1}) + (b_i - b_{i-1})] \tag{11}$$

One sees immediately that a difference of 1 between a_i and a_{i-1} implies the presence of the number i twice in the corresponding Weyl tableau. Similarly, a difference of 1 between b_i and b_{i-1} must imply the presence of the number i once in the Weyl tableau. Thus, the value of the matrix element is merely the number of times the entry i occurs in the Weyl tableau:

$$\langle m|E_{ii}|m'\rangle = \delta_{mm'}(n_{x_i} + n_{y_i}) \tag{12}$$

where $n_{x_i}=1$ if $x_i=i$ and 0 otherwise and similarly for n_{y_i}.

5. Basis Vector Generation in Total Weight Form

The starting point in the Weyl and Gelfand branching methods is the highest weight tableau. In terms of Gelfand tableaux the highest weight tableau is the one for which the numbers in the columns of the Gelfand tableau do not increase when reading from bottom to top (i.e. $m_{ai}=m_{an}$ for all i for a given column a). Accordingly the Weyl tableau corresponding to this situation consists simply of a first row contains 1's, a second row contains 2's etc. This remains true regardless of the orbital space in which the representation exists. In terms of the Weyl line tableau

(8) the highest weight will consist of a single row of numbers x_i increasing monotonically in unit steps until the length of the first column is reached and similarly for the second column. For example

$$|m\rangle_{hw}=|1, 2, 3, \ldots, t; 1, 2, 3, \ldots, u\rangle \tag{13}$$

It is now convenient to define the total weight T of a Weyl tableau as the sum of the numbers in the tableau:

$$T=\sum_i^t x_i+\sum_i^u y_i. \tag{14}$$

There will in general be several tableaux having the same total weight but there will only be one having the total weight T_1 of the highest weight tableau[1] in the Gelfand scheme. Since this unique tableau is easily found it is the natural starting point from which to derive all other tableaux. We can systematically find all the tableaux of next highest total weight T_2 by increasing each of the numbers in the Weyl tableau by 1 and testing for the Weyl standardness condition (i.e. the numbers in any row or column must not decrease and the same number cannot occur twice in a column).

In this way one can find several tableaux of the form

$$|x_1, x_2, \ldots, x_r+1, \ldots, x_t; y_1, y_2, \ldots, y_u\rangle$$

from the highest weight tableau. However, one immediately observes the relation between this tableau and the one from which it was generated

$$|x_1, x_2, \ldots, x_r, \ldots, x_t; y_1, y_2, \ldots, y_t\rangle$$

corresponds exactly to the condition (9b) for a matrix element of the elementary generator E_{x_r, x_r+1}. Thus if we generate the basis tableau of the total weight T_{p+1} from those of the weight T_p in the manner just suggested we have the possibility of simultaneously calculating the value of the matrix elements of the generators.

Since we are concerned only with the elementary raising generators we can be sure that the above mentioned scheme will generate all possibilities. A Weyl tableau $|\ldots j \ldots\rangle$ of total weight T_{p+1} is obviously related by the elementary generator E_{ij} to a Weyl tableau $|\ldots i \ldots\rangle$ of total weight T_p for $j=i+1$. Further, the basis vectors of total weight T_{p+2} can only be related by the elementary raising operator to those of T_{p+1} and so on. From a practical point of view this scheme will be highly efficient since once the vectors of weight T_{p+1} have been found and the possible matrix elements with the vectors of weight T_p have been computed, the vectors for T_p can be discarded before generating those of weight T_{p+2}. Because the number of basis vectors of a given total weight T_p increases much more slowly than the

[1] To avoid confusion it should be pointed out that the notion of weight within the Gelfand scheme refers to the eigenvalues of the E_{ii} generators. Thus the total weight T_1 of the highest weight Gelfand state is actually the lowest total weight of T_m of all the possible Gelfand states.

dimension of the irreducible representations in $U(n)$ the scheme is computationally attractive in the case where the number of electrons is small and the orbital basis (n) is large and thus no possibility of holding all the basis vectors in high speed computer memory.

There is, however, a small complication in the above scheme when deriving the basis vector of a total weight T_{p+1} from those of total weight T_p when there are several vectors of weight T_p (as is generally the case). For example a basis vector with the same T_3 total weight could be produced from two different T_2 basis vectors by the two routes

$$|x_1 \ldots x_r+1 \ldots x_s \ldots x_t;\, y_1 \ldots y_u\rangle \rightarrow |x_1 \ldots x_r+1 \ldots x_s+1 \ldots x_t; y_1 \ldots y_u\rangle \tag{15}$$

$$|x_1 \ldots x_r \ldots x_s+1 \ldots x_t; y_1 \ldots y_u\rangle \rightarrow |x_1 \ldots x_r+1 \ldots x_s+1 \ldots x_t; y_1 \ldots y_u\rangle \tag{16}$$

Thus a given basis vector in T_3 obtained from one in T_2 may have already been obtained from a different T_2 basis function so it must be checked against the current list of T_3 basis vectors before being added to the list. However, even though both the basis vectors generated under the above conditions do not lead to distinct states, they do give distinct matrix elements, the first in E_{x_s, x_s+1} the second in E_{x_r, x_r+1}. Consequently, we automatically obtain all non-zero elementary generator matrix elements as we generate basis vectors by total weight.

Raising generators other than the elementary generators are obtained by matrix multiplication through the use of Eq. (5b). Here, again we obtain considerable simplification if the basis vectors have been generated by total weight T_p. For example, the first E_{ps} of Eq. (5b) to be found would be $E_{p,p+2}$ and these generators would only have matrix elements between basis vectors with weights T_p and T_{p+2}. In other words the vast majority of matrix elements will be zero in principle and only those related via total weights as above need to be considered. A similar situation is encountered (but less obviously) when the product matrices $E_{pq}E_{rs}$ are computed. (These products are required for the computation of the matrix representative of the Hamiltonian which is bilinear in the generators.) For example, if E_{pq} is the raising operator $E_{p,p+2}$ and E_{rs} is the raising operator $E_{r,r+3}$, then there are only matrix elements of the product between basis states of weights T_p and T_{p+5}.

6. An Example: The Irreducible Representation [2, 1, 1, 0] in U(4)

The above ideas are perhaps best illustrated with a non-trivial but simple example: the representation [2, 1, 1, 0] in $U(4)$.

The first step is the calculation of the range of total weights. The Weyl tableau corresponding to the highest weight Gelfand tableau [2, 1, 1, 0] has the form $|123; 1\rangle$ in the notation of Eq. (8) and its total weight is T_7. The lowest weight Gelfand tableau gives the Weyl tableau $|234; 4\rangle$ and corresponds to total weight T_{13}. The basis vectors of total weight T_8 are obtained as

$$^{1}|123;1\rangle \quad 3\rightarrow 4 \quad ^{2}|124;1\rangle \tag{17}$$

$$^{1}|123;1\rangle \quad 1\rightarrow 2 \quad ^{3}|123;2\rangle \tag{18}$$

Basis vector 2 is thus obtained from 1 by increasing 3 to 4. Consequently the E_{34} generator has a (1, 2) matrix element given by Eqs. (7b) and (10). Only basis vector 2 is needed to compute the matrix element once the fact that the matrix element is of type B is observed. Since $i=3$ the b_l values needed are b_2, b_3 and b_4 which have values 1, 1 and 2 respectively. The (1, 2) matrix element of E_{34} is thus 1. Similarly, basis vector 3 gives rise to a (1, 3) matrix element of the E_{12} generator which is of A type (Eq. (7a)). The b_l required are b_0, b_1 and b_2 which have values 0, 1 and 1 respectively giving a final matrix element of 1. Note that all other possible increases violate the standardness conditions for Weyl tableaux.

The full set of basis vectors for the problem is illustrated in Fig. 2 and the matrix elements for the elementary raising operators are collected in Fig. 3. There are 22

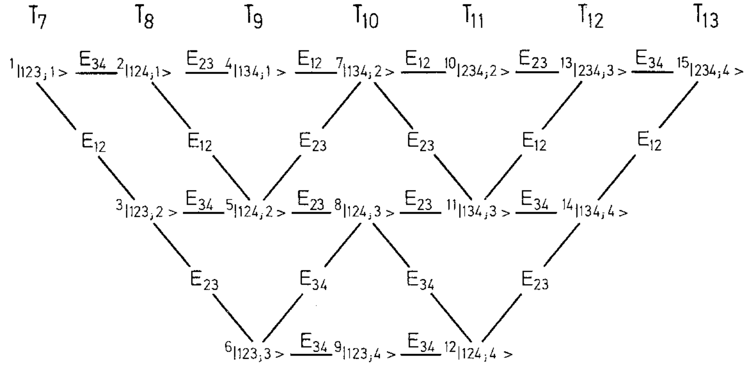

Fig. 2. Basis vectors for representation [2,1,1,0] of $U(4)$ in total weight order

	m_1	m_2	m_3	m_4	m_5	m_6	m_7	m_8	m_9	m_{10}	m_{11}	m_{12}	m_{13}	m_{14}	m_{15}
m_1		$1^{(34)}$	$1^{(12)}$												
m_2				$1^{(23)}$	$1^{(12)}$										
m_3					$1^{(34)}$	$1^{(23)}$									
m_4							$1.414^{(12)}$								
m_5							$0.707^{(23)}$	$1.224^{(23)}$							
m_6								$0.816^{(34)}$	$1.154^{(34)}$						
m_7										$1.414^{(12)}$	$0.707^{(23)}$				
m_8											$1.224^{(23)}$	$0.816^{(34)}$			
m_9												$1.154^{(34)}$			
m_{10}													$1^{(23)}$		
m_{11}													$1^{(12)}$	$1^{(12)}$	
m_{12}														$1^{(23)}$	
m_{13}															$1^{(34)}$
m_{14}															$1^{(12)}$
m_{15}															

Fig. 3. Matrix elements of the elementary generators of $U(4)$ for representation [2,1,1,0]

"tie" lines in Fig. 2 connecting basis functions having integer difference between standard tableaux. The "tie" lines represent the possible ways of generating functions of total weight T_{p+1} from those of weight T_p. There are thus 22 non-zero matrix elements of the elementary raising generators E_{12} E_{23} and E_{34} and these are collected in Fig. 3. The entries are denoted $(Z^{(E_{ij})})_{m_k, m_l}$ where Z is the numerical value of the m_k, m_l element of generator E_{ij}. Note that because of the matrix element relationships between two tableaux the matrix elements of the different basis generators can never occur in the same position.

Finally, the matrix elements of the weight generators E_{ii} are readily found from Eq. (12). Thus

$$\langle 123;\, 1|\mathrm{E}_{ii}|123;\, 1\rangle = \begin{cases} 2 & \text{for } i=1 \\ 1 & \text{for } i=2 \text{ or } 3. \end{cases}$$

7. Comparison with the "Harmonic Excitation Diagram" and Δac Tableau Methods of Paldus

After this work was complete the authors became aware of more recent work of Paldus [8] in which the generation of basis functions by total weight is described by "harmonic excitation diagrams". In Paldus' work the information shown in Fig. 2 is presented in the form of a two-rooted graph[2] where the roots are the minimal and maximal states. The T_p-level states are represented by the T_p-level verticies and the diagram is obtained with only first level edges (representing the elementary generator matrices elements). As Paldus [8] points out the verticies may be labelled arbitrarily so that this method is identical to the scheme described in Sect. 5. Also we should add that a similar scheme has been discussed by Harter and Patterson [9].

From the point of view of computational implementation of Unitary Group methods it should be pointed out that the methods discussed in Paldus' [1] original paper are not really suitable as actual computational algorithms, but rather serve to illustrate the structure of the general theory. In more recent work [2, 3, 8, 10], Paldus has developed a representation of the Gelfand states by Δac tableaux (the first difference tableau of the "a" and "c" columns of the tableau in Eq. (6).) This representation is particularly suitable for computation since each state is represented by two binary strings of length n. In this representation the matrix element formulae are simplified (c.f. Eqs. (21) and (22) of Ref. [10]) and the relationship between the Weyl tableaux and Gelfand tableaux becomes straightforward. In particular we should point out that formula (10) in this work is easily related to formula (29) in Ref. [9] using the Δac tableau method.

The methods discussed in this work are easily implemented in terms of the Δac tableaux and the example presented in Fig. 2 is given again in terms of the Δac

[2] It should be noted that the two-rooted graph shown in Fig. 2 is different than the one discussed briefly by Paldus [3] or in the recent elegant graphical analysis by Shavitt [14].

tableau in Fig. 4. In this representation, it can be seen that the action of an elementary generator merely exchange an adjacent "1" and "0" in one of the columns where the row labels correspond to the subscripts of the generator (note that the rows are numbered from the bottom of the tableau). The total weights are easily identified by taking the binary ones complement of the second column whence the number of 1's in a row of the resultant tableau gives the occupation number of the corresponding orbital.

8. Discussion

Although Paldus [3] has developed a method for the direct calculation of the non-elementary generators of $U(N)$, the direct method will probably be less efficient than one based on Eq. (5b) in most circumstances (see the discussion in Ref. [8]). It is in the evaluation of the products of generators occurring in Eq. (5b) and in the evaluation of the bilinear terms in the Hamiltonian that the total weight order of the basis functions becomes preferred over the canonical Gelfand order. The non-elementary generators take on a simple block structure by total weight (e.g. $E_{p,p+q}$ has matrix elements only between basis vectors whose total weight differs by q). Thus one has "selection rules" that enable the efficient evaluation of the bilinear part of the Hamiltonian.

With a view to applications in atomic physics, when we are concerned with $U(2l+1)$ for shell of quantum number l, it is clear that the total weight T_p is related to the azimuthal quantum number M_z by the addition of a constant. Thus applications involving electronic angular momentum require basis vectors in the order in which we derive them [5, 6, 9, 11]. For example, the L^2 operator

$$(L_Z^2 - L_+L_- - L_-L_+)$$

has non-zero matrix elements only between basis vectors of the same total weight. (This follows directly from the fact that L_+ and L_- are linear combinations of elementary raising and lowering generators).

In application of the unitary group approach to CI calculations one will often be forced to truncate the basis at say quadruple replacements with respect to some dominant configuration. In the present method, basis vectors can be rejected according to the truncated requirement[3] at the point of generation and thus one has the advantage that basis vectors of higher total weight which would have to be rejected in the Gelfand canonical basis are in fact never created. In addition as discussed by Paldus [8] the present type of scheme may also prove to be useful in the so called "direct" CI method (see Ref. [12] for example).

Clearly, it would be desirable to have an algorithm for obtaining the elementary generators without explicitly generating the basis. Paldus [13] has in fact derived such a method using a graphical representation of the Δac tableaux. Since, in most

[3] In the evaluation of the bilinear part of the Hamiltonian, one must keep intermediate states one excitation level higher than one's ultimate truncation requirement.

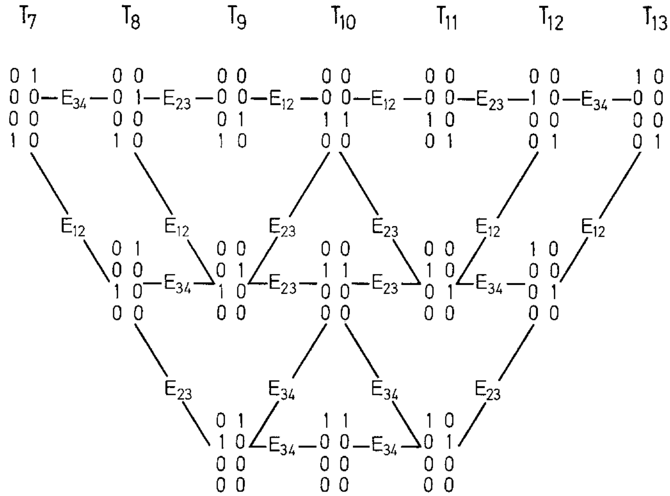

Fig. 4. Basis vectors for representation [2,1,1,0] of $U(4)$ in total weight order in the Δac tableau representation

applications one will want to truncate the CI expansion one will probably wish to generate the basis vectors explicitly. In this case, basis generation by total weight is to be preferred since one need only keep basis vectors of weight T_p and T_{p+1} at any stage in the computation.

In the actual computation of the matrix elements of the elementary generators for two sets of basis vectors of weight T_p and T_{p+1} there are two problems which govern the efficiency of the method. Firstly, in generating a vector of weight T_{p+1} from one of weight T_p one must search for the standardness conditions of the Weyl tableau. While this requires only a few logical operations, it is clear that the Δac tableau would have advantages at this point. Secondly, one has the problem of searching the list of basis vectors of weight T_{p+1} for duplicate entries as each basis vector is generated. However, this search is facilitated if the basis vectors are generated by allowing all the elementary generators to operate, in succession, on the first column of a Weyl tableau of weight T_p and then allowing all the generators to operate on the second column. The basis vectors of each weight will then be generated in "page order" if the line tableau is read from left to right. Thus the appearance of a basis vector that has been generated previously is easily recognizable as being out of sequence and one has only to search the list backwards to pick up the correct sequence number of this duplicate vector. The corresponding Δac tableaux are also obtained in page order if the Δax and Δc columns are written consecutively and read from left to right as a binary integer. This is the method used

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