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The evaluation of matrix elements for non-canonical Weyl tableau basis states adapted to $U(n_1+n_2) \supset U(n_1) \times U(n_2)$

I. Explicit formulae for subduction coefficients

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Summary. This is the first paper of a series of two, which enables the evaluation of $U(n)$ generator matrix elements in the non-canonical Weyl tableau basis adapted to subgroup $U(n_1) \times U(n_2)$. In this paper the explicit closed formulae for subduction coefficients are presented. These formulae will become useful through an inductive method to be presented in the second paper.

Key words: Weyl tableau – Subduction coefficients – Matrix elements

1. Introduction

One of the most promising ideas from group theoretical approaches to the molecular configuration interaction (CI) problem advanced during last decades is the unitary group approach (UGA) [1–6]. It is not only a mathematically beautiful formalism but also a practical and powerful tool both for basis generation and evaluation of generator matrix elements. Many of the UGA developments up to 1986 have been summarized by Matsen and Pauncz [7].

The molecular configuration interaction problem quickly becomes unwieldy with increasing numbers of electrons and basis orbitals. It is thus desirable to have a unitary group approach formalism giving a general partitioning of the system. The essential idea is to consider the following subgroup imbedding

$$U(n = n_1 + n_2) \supset U(n_1) \times U(n_2). \tag{1}$$

Recently, a complete derivation of the $U(n)$ generator matrix elements in the non-canonical bases adapted to the group chain (1) was presented by Gould and Paldus [8] from the viewpoint of the Green–Gould characteristic identities for $GL(n)$ [9]. Another traditional method of evaluating the $U(n)$ generator matrix elements in the non-canonical bases is by means of the subduction coefficients of group chain (1), which has previously been considered by Harter and Patterson [10]. This method, however, is rather complicated, because a lot of matrix elements in the canonical bases need to be calculated even in very simple cases.

It is our aim in the present series of two papers to offer a new idea, which significantly improves the traditional method. We shall examine the problem of evaluating the matrix elements of the $U(n)$ generators in the non-canonical Weyl tableau basis, which is symmetry adapted to the subgroup chain (1), by means of the method developed in [11]. That method enabled the evaluation of the $U(2n)$ generator matrix elements in the Weyl tableau basis adapted to subgroup $U(2) \times U(n)$. As the first step, we evaluate subduction coefficients of group chain (1).

There have been many attempts to calculate the unitary group subduction coefficients. Patterson and Harter [10] derived recursive formulae for the $U(n) \supset U(n_1) \times U(n_2)$ subduction coefficients by the use of spin algebras. Later, Wen [12] translated the formulae into spin graphical formulae. Using the transformation properties of the tensor basis spanning the irreducible representation $[2^{N/2-S}, 1^{2S}]$ of $U(n)$ under the permutations of electron coordinates, Sarma and Dinesha [13] obtained relations among the coefficients in a given set, which can be determined by the normalization requirement. Recently, Paldus et al. [14] presented a method to determine the subduction coefficients of the Weyl tableau bases. We shall derive, in this paper, explicit closed formulae for arbitrary subduction coefficients in terms of the isoscalar factors and the l-particle coupling formulae, which are essential for the developments in the second paper of this series.

2. Notation and fundamentals

We assume that an n-dimensional orbital space V can be partitioned into the direct sum of subspaces V_1 and V_2 with dimensions n_1 and n_2, respectively, so that

$$V = V_1 \oplus V_2$$

$$n = n_1 + n_2. \tag{2}$$

For convenience, we always assume that the orbital order in subspace V_1 is $1, 2, \ldots, n_1$, and that in V_2 is $n_1+1, n_1+2, \ldots, n_1+n_2$. Generally, we shall thus associate with the orbital space V the unitary group $U(n)$, as well as with each orbital subspace V_i the unitary group $U(n_i)$. Now let $\left|\begin{matrix}[V_i]\\ W_i\end{matrix}\right\rangle$ (or $|W_i\rangle$) be the Weyl tableau basis spanning the irreducible representation (IR) $[V_i]$ of subgroup $U(n_i)$, then the non-canonical Weyl tableau basis adapted to the subgroup $U(n_1) \times U(n_2)$ for the $IR[V] = [2^{N/2-S}, 1^{2S}]$ of $U(n)$ can be denoted as $\left|\begin{matrix}[V];[V_1][V_2]\\ W_1 W_2\end{matrix}\right\rangle$, where N is the total number of electrons in the system, and S is the total spin quantum number.

Further, let $\left|\begin{matrix}[V]\\ W\end{matrix}\right\rangle$ (or $|W\rangle$) be the canonical Weyl tableau basis adapted to the canonical subgroup chain

$$U(n) \supset U(n-1) \supset \cdots \supset U(1) \tag{3}$$

for the $IR[V]$ of $U(n)$. Then, the transformation between the canonical and non-canonical Weyl tableau basis sets is given by the following relation

$$\left|\begin{matrix}[V];[V_1][V_2]\\ W_1 W_2\end{matrix}\right\rangle = \sum_W \left|\begin{matrix}[V]\\ W\end{matrix}\right\rangle \cdot \left\langle\begin{matrix}[V]\\ W\end{matrix}\right|\left.\begin{matrix}[V_1][V_2]\\ W_1 W_2\end{matrix}\right\rangle \tag{4}$$

where

$$\left\langle\begin{matrix}[V]\\ W\end{matrix}\right|\left.\begin{matrix}[V_1][V_2]\\ W_1 W_2\end{matrix}\right\rangle \tag{5}$$

is a subduction coefficient, and the multiplicity indices are dropped, since they will not be required for the case of many-electron systems.

At first, we recall the basic fact: if $|W\rangle/|W_2\rangle$ denotes the skew part in the $|W\rangle$ found by removing the boxes belonging to $|W_2\rangle$ from $|W\rangle$, then the necessary condition for the subduction coefficients being non-zero is that

$$|W_1\rangle = |W\rangle/|W_2\rangle. \tag{6}$$

Furthermore, the subduction coefficient (5) is independent of the actual Weyl tableau basis of $|W_1\rangle$. From now on, we assume that Eq. (6) is always satisfied.

In general, the subduction coefficients are real and they satisfy the following orthogonality relations

$$\sum_{V_1,V_2,W_1,W_2} \left\langle \begin{matrix}[V] \\ W\end{matrix} \middle| \begin{matrix}[V_1][V_2] \\ W_1\, W_2\end{matrix} \right\rangle \left\langle \begin{matrix}[V_1][V_2] \\ W_1\, W_2\end{matrix} \middle| \begin{matrix}[V] \\ W'\end{matrix} \right\rangle = \delta_{W,W'} \tag{7}$$

$$\sum_{W} \left\langle \begin{matrix}[V] \\ W\end{matrix} \middle| \begin{matrix}[V_1][V_2] \\ W_1\;\; W_2\end{matrix} \right\rangle \left\langle \begin{matrix}[V_1'][V_2'] \\ W_2'\;\; W_2\end{matrix} \middle| \begin{matrix}[V] \\ W\end{matrix} \right\rangle = \delta_{V_1,V_1'}\delta_{V_2,V_2'}\delta_{W_1,W_1'}\delta_{W_2,W_2'}. \tag{8}$$

From given $[V_1]$ and $[V_2]$, all the $[V]$ which satisfy the relation

$$[V_1] \times [V_2] \supset [V] \tag{9}$$

can be determined by the Littlewood–Richardson rules. In the simplest case of a many-electron system, these rules are the same as the rules of angular momentum coupling. Namely, if we introduce

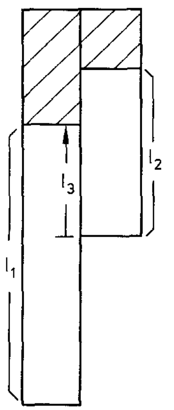
$$\Delta S = S_1 + S_2 - S \tag{10}$$

where $S(S_i)$ is the spin quantum number of $IR[V]([V_i])$, then relation (9) corresponds to

$$\begin{aligned} \Delta S &= 0, 1, 2, \ldots, d_2 - 1 \quad \text{for } d_2 \leqslant d_1 \\ \Delta S &= 0, 1, 2, \ldots, d_1 - 1 \quad \text{for } d_2 > d_1 \end{aligned} \tag{11}$$

where d_i denotes the axial distance (without direction) between the last box of each column in Young diagram $[V_i]$. The axial distance is a very important concept in our approach where all the formulae contain this quantity [1].

All the $[V_2]$, which will satisfy relation (9) for given $[V]$ and $[V_1]$ can be determined by the division rules of Young diagrams [6]. In the case of a Young diagram with at most two columns:



where the shaded part refers to $[V_1]$ and the total one refers to $[V]$, the Young diagram of $[V_2]$ should satisfy the relation

$$\max(l_3, 0) \leqslant \lambda_2 \leqslant \min(l_1, l_2) \tag{12}$$

where λ_2 is the box-number in the second column of $[V_2]$, and l_i are the box-numbers indicated in the above diagram (note: l_3 has a direction or sign). It is obvious that those $[V_2]$ satisfying the angular momentum coupling relation are not allowed if $l_3 < 0$ because of the limitation of the number of electrons.

Finally, relations (11) or (12) are necessary constraints, as they are the selection rules for the subduction coefficients being non-zero.

3. Explicit expressions for subduction coefficients

It is well-known [15] that the $U(n_1 + t)$ subduction coefficient can be factored into a product of the $U(n_1 + t - 1)$ subduction coefficient and the isoscalar factor R_t,

$$\left\langle \begin{matrix} [V_{n_1+t}] \\ W_{n_1+t} \end{matrix} \middle| \begin{matrix} [V_{n_1}][V_t] \\ W_{n_1} W_t \end{matrix} \right\rangle = R_t \left\langle \begin{matrix} [V_{n_1+t-1}] \\ W_{n_1+t-1} \end{matrix} \middle| \begin{matrix} [V_{n_1}][V_{t-1}] \\ W_{n_1} W_{t-1} \end{matrix} \right\rangle \tag{13}$$

where

$$R_t = \left[\begin{matrix} [V_{n_1+t}] \\ [V_{n_1+t-1}] \end{matrix} \middle| \begin{matrix} [V_{n_1}][V_t] \\ [V_{t-1}] \end{matrix} \right]. \tag{14}$$

It is important to note that the isoscalar factor R_t is independent of the Weyl tableau basis structure of the $[IR]$ of the canonical subgroup $U(n_1 + t - 1)$ and of the non-canonical subgroup $U(t - 1)$.

Finally, the group $U(n = n_1 + n_2)$ subduction coefficient can be expressed as a product of isoscalar factors by applying (13) recursively, namely,

$$\left\langle \begin{matrix} [V_n] \\ W_n \end{matrix} \middle| \begin{matrix} [V_{n_1}][V_{n_2}] \\ W_{n_1} W_{n_2} \end{matrix} \right\rangle = \prod_{t=1}^{n_2} \left[\begin{matrix} [V_{n_1+t}] \\ [V_{n_1+t-1}] \end{matrix} \middle| \begin{matrix} [V_{n_1}][V_t] \\ [V_{t-1}] \end{matrix} \right] = \prod_{t=1}^{n_2} R_t. \tag{15}$$

For $t = 1$, we have

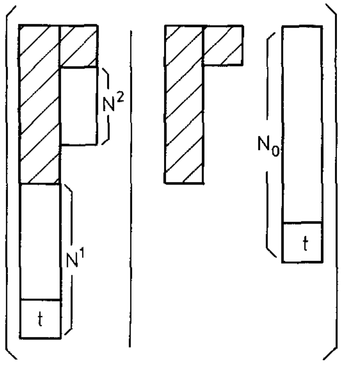
$$R_1 = 1. \tag{16}$$

We shall now derive closed formulae for the isoscalar factor. According to the relations (4) and (13) for the subduction and isoscalar factors, we immediately obtain

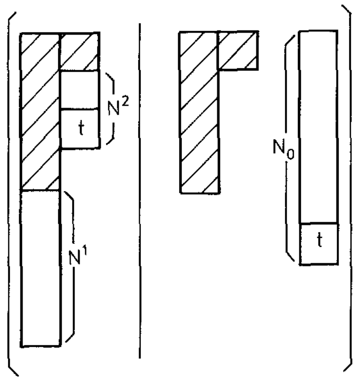
$$\left[\begin{matrix} [V_{n_1+t}] \\ [V_{n_1+t-1}] \end{matrix} \middle| \begin{matrix} [V_{n_1}][V_t] \\ [V_{t-1}] \end{matrix} \right] = 1 \quad \text{for } N_{n_1+t} = 0, 2 \tag{17}$$

where N_{n_1+t} is the occupancy of the $(n_1 + t)$th orbital in the space V, in other words, that of the t-th orbital in the subspace V_2.

From Eq. (59) of [14], it is easy to obtain the expressions for the two following special isoscalar factors:



$$= \sqrt{\frac{N^1}{N_0}} \cdot \sqrt{\frac{d+N^2}{d}} \tag{18}$$

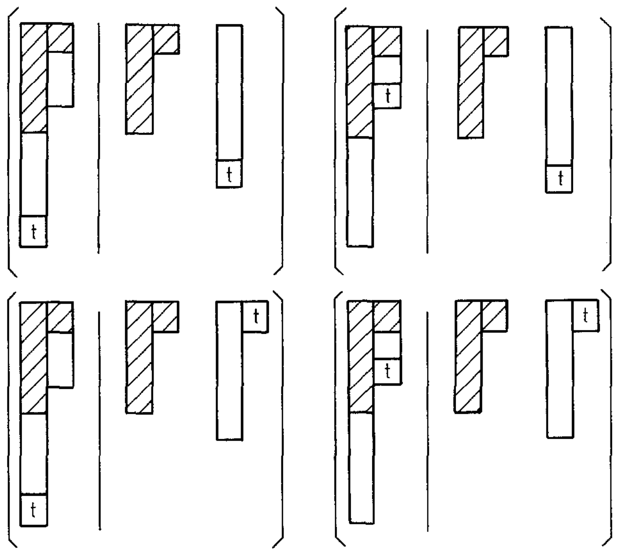


$$= (-1)^{N^1} \sqrt{\frac{N^2}{N_0}} \cdot \sqrt{\frac{d-N^1}{d}}. \tag{19}$$

It should be pointed out that in [14] only the highest weight Weyl tableau bases were needed. However, it is now obvious that the conclusions are also correct for the special case $[V_t] = [1^m]$.

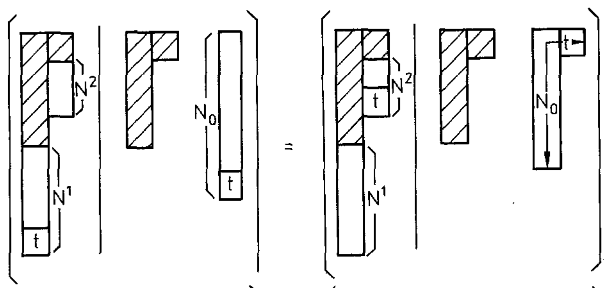
In Eqs. (18–19) the explicit schematic expressions for the isoscalar factor are used, and the symbol d denotes the axial distance between the last box of each column in $[V_{n_1+t}]$, and N_0, N^1, N^2 ($N_0 = N^1 + N^2$) denote the number of boxes as shown in the figure. It is obvious that Eqs. (18–19) satisfy the normalization condition.

From the orthogonality relations of Eqs. (7–8), one can derive the following four R_t, which, possessing the same $[V_{n_1+t}]$, $[V_{n_1}]$ and $[V_{t-1}]$, are elements of a unitary matrix:

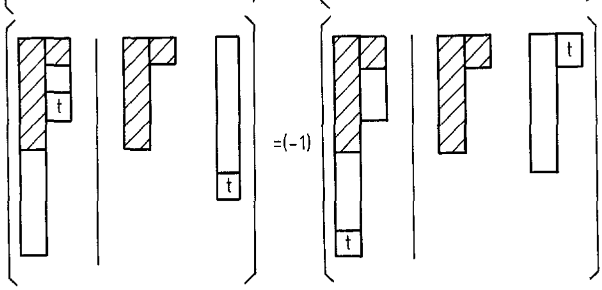


(20)

Combining Eqs. (18) and (19), we obtain



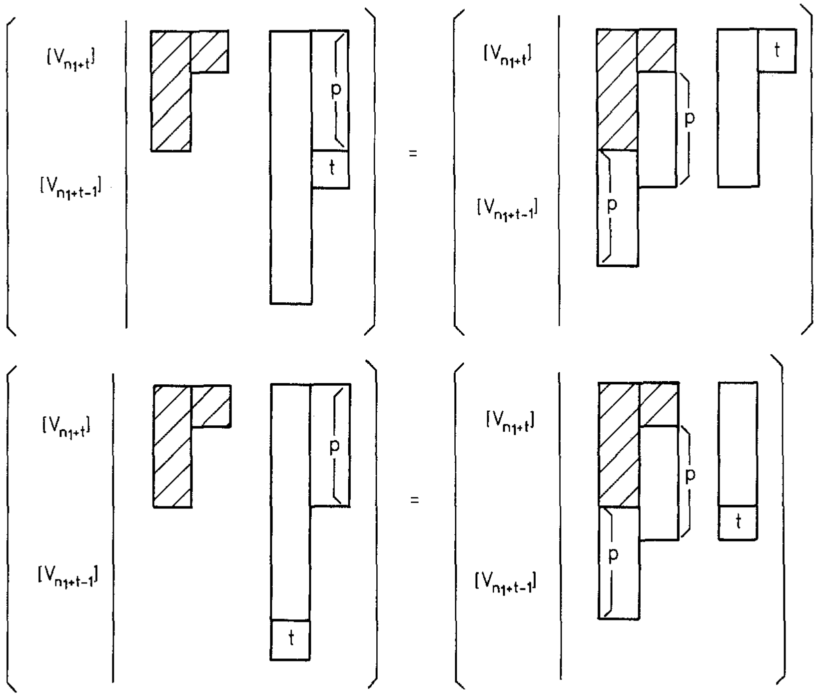
$$= \sqrt{\frac{N^1}{N_0}}\sqrt{\frac{d+N^2}{d}} \tag{21}$$



$$= (-1)^{N^1}\sqrt{\frac{N^2}{N_0}}\sqrt{\frac{d-N^1}{d}} \tag{22}$$

where the phase was chosen so that the elementary generator matrix elements are always positive.

For the more general case, where $[V_t]$ is an arbitrary Young diagram, noting that R_t is independent of the Weyl tableau basis structure of the $IR[V_{t-1}]$, we can get an interesting and useful property of the isoscalar factor, namely,



(23)

Equation (23) can be obtained by virture of a special Weyl tableau basis where each of the first P rows consists of the same integer.

So far, the expressions for all R_t have been obtained. In order to illustrate the application of these formulae, an example for the evaluation of the subduction coefficient for $U(8) \supset U(2) \times U(6)$ is shown here.

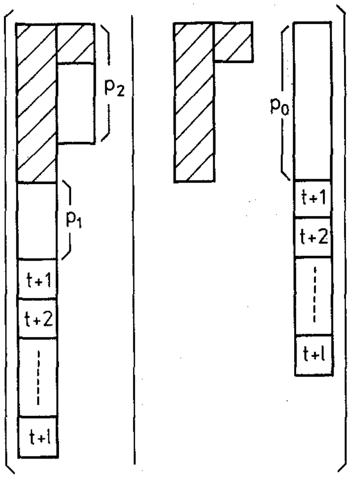
$$\left\langle \begin{array}{cc|cccc} 1 & 2 & 1 & 2 & 3 & 4 \\ 2 & 4 & 2 & & 4 & 7 \\ 3 & 6 & & & 5 & \\ 4 & 8 & & & 6 & \\ 5 & & & & 8 & \\ 7 & & & & & \end{array} \right\rangle$$

$$= \prod_{t=1}^{6} R_t = (1) \cdot (1) \cdot \left[\sqrt{\frac{2 \cdot 4}{2 \cdot 4}}\right] \cdot \left[(-1)^2 \cdot \sqrt{\frac{1 \cdot (3-2)}{3 \cdot 3}}\right]$$

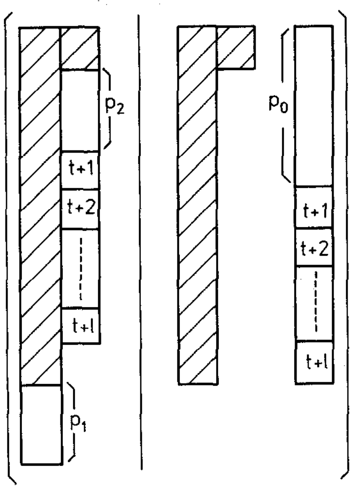
$$\cdot \left[(-1)^4 \cdot \sqrt{\frac{1 \cdot (4-3)}{4 \cdot 4}}\right] \cdot \left[(-1)^2 \cdot \sqrt{\frac{1 \cdot (3-2)}{3 \cdot 3}}\right]$$

$$= 1 \cdot 1 \cdot 1 \cdot \frac{1}{3} \cdot \frac{1}{4} \cdot \frac{1}{3} = \frac{1}{36}.$$

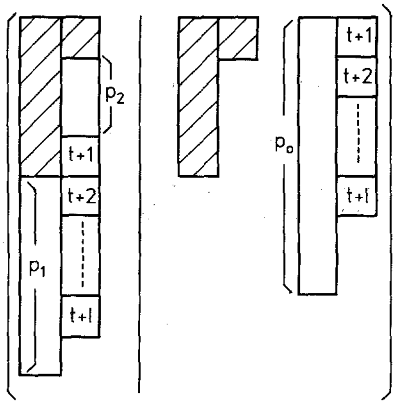
Now we go a step further and consider the situation where l-particles $t+1, t+2, \ldots, t+l$ couple to $|W_t\rangle$ as an ensemble. This will be useful for part II of the present work. Then, instead of Eqs. (21–22), the following expressions are obtained by a consecutive application of preceding rules:



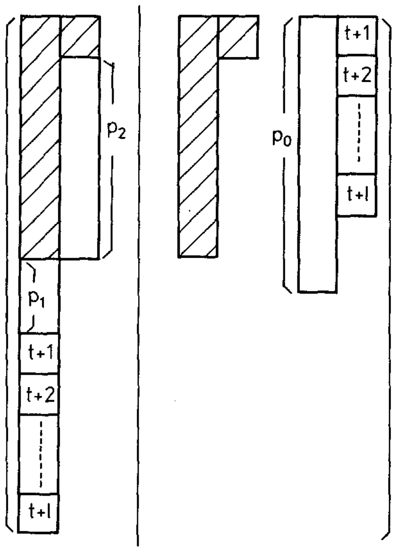
$$= \sqrt{\frac{P_0!(P_1+l)!d!(d+P_2+l)!}{P_1!(P_0+l)!(d+P_2)!(d+l)!}} \tag{24}$$



$$= (-1)^{lP_1} \sqrt{\frac{P_0!(P_2+l)!(d-P_1-1)!(d-1-l)!}{P_2!(P_0+l)!(d-P_1-1-l)!(d-1)!}} \tag{25}$$



$$= \sqrt{\frac{P_1!(P_0 - l + 1)!(d + P_2)!(d - 1 - l)!}{(P_0 + 1)!(P_1 - l)!(d - 1)!(d + P_2 - l)!}} \tag{26}$$



$$= (-1)^{lP_1} \sqrt{\frac{P_2!(P_0 - l + 1)!(d - P_1 + l - 1)!d!}{(P_0 + 1)!(P_2 - l)!(d + l)!(d - P_1 - 1)!}} \tag{27}$$

In Eqs. (24–27) the parameters P_i and d refer to the case before coupling, P_i ($P_0 = P_1 + P_2$) are the number of boxes as shown in the figures, and d is the axial distance between the last box of each column of the canonical basis before the l-particles have been coupled.

It is worthwhile to mention that the results are zero if a factorial of a negative integer appears. This reflects the fact that the selection rules of Eqs. (11) or (12) are not satisfied.

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