Unitary-group approach to the many-electron correlation problem: Relation of Gelfand and Weyl tableau formulations*

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The recent electronic orbital tableau ("jawbone") formulas of Harter and Patterson for matrix representatives of elementary generators of $U(n)$ in the canonical basis are shown to be simply related to our expressions for the latter, which are based on a simplified Gelfand tableau formalism pertinent to N-electron problems, a brief survey of which is given in a form particularly suitable for computer implementation.

I. INTRODUCTION

Many different approaches exist to basic problems of shell-model (configuration interaction) calculations: a construction of (permutation, spin, isospin, space, etc.) symmetry-adapted N-fermion bases and a calculation of pertinent matrix representatives of observables in these bases. One of the most mathematically appealing and computationally efficient approaches, due to Moshinsky,[1] is based on the unitary-group representation theory. While some fundamental ideas of this approach were already pointed out by Jordan,[2] it is remarkable that the necessary mathematical machinery was only sufficiently developed much later by Gelfand *et al.*,[3] Moshinsky *et al.*,[4] Biedenharn *et al.*,[5] Louck *et al.*[6] and others, extending thus the classical works of Weyl,[7] Cartan, Casimir, Killing, and others (cf. for example Ref. 8).

Recently, there has been a renewed interest in this and similar approaches[9-25] in connection with large-scale molecular configuration-interaction (shell-model) calculations.[26] It was found that for systems of identical fermions with only one dichotomic internal degree of freedom (e.g., electrons) the relevant formalism may be drastically simplified and efficient algorithms formulated.[14,19,22] While our approach[14,19,24] exploits a simplified Gelfand tableau formalism, Harter and Patterson published recently[22,23] and algorithm based on Weyl tableaus, which they deem preferable for practical applications.

It is the purpose of this paper to show the equivalence and mutual relationship of both algorithms, however differently they may look at first sight. Indeed, we shall establish a very simple and direct relationship between our simplified electronic Gelfand tableaus and the corresponding Weyl tableaus, which in turn yield Harter and Patterson's tableau formulas[22,23] from our unified algebraic[14,19,24] (or, equivalently, pattern[19,24]) formulas. Out of several formulations which we used earlier to present our approach, we choose here the most suitable one for computer implementation.

II. BASIC FORMALISM AND NOTATION

In configuration-interaction calculations for N-electron systems described by a spin-independent model Hamiltonian,[27] we are faced with the following problems: (i) find a spin-symmetry-adapted basis (preferably orthonormal) in a totally antisymmetric component of the Nth rank tensor product space $\mathfrak{V}^{\otimes N}$ of finite-dimensional one-particle spaces $\mathfrak{V}$ ($\dim\mathfrak{V}=n\geq N$), on which the model Hamiltonian is defined, and (ii) determine the matrix representative of the Hamiltonian (and, if desired, of other observables) in this basis.

The individual spin-invariant subspaces may be conveniently labeled by the pertinent eigenvalues of the total spin operators, $\hat{S}^2$ and $\hat{S}_z$ and, in view of the spin independence of forces considered, we can limit ourselves to one particular eigenvalue S_z of $\hat{S}_z$, say $S_z=S$.

As Moshinsky[1] has shown, a convenient choice of such a spin-adapted basis, for a subspace characterized by the total spin quantum number S, is supplied by the Gelfand-Tsetlin canonical basis[3] for the carrier space of the irreducible representation (irrep) $\Gamma\{2^{N/2-S}1^{2S}\}$ of $U(n)$. The individual basis vectors (i.e., the N-electron spin-adapted configuration-state functions) are then uniquely labeled by the Gelfand tableaus $[\underline{m}]$,

$$[\underline{m}]=\begin{bmatrix} m_{1n} & m_{2n} & \cdots & & & m_{nn} \\ & m_{1,n-1} & \cdots & & m_{n-1,n-1} & \\ & & \cdots & & & \\ & & & m_{12} & m_{22} & \\ & & & & m_{11} & \end{bmatrix}, \quad (1)$$

whose integer entries m_{ij} ($i\leq j$; $j=1,2,\ldots,n$; $m_{ij}\in Z$), satisfy the so called "betweenness conditions" (lexical tableaus)

$$m_{i,j+1} \geq m_{ij} \geq m_{i+1,j+1} \tag{2}$$

and whose first row $[\underline{m}_n]$,

$$[\underline{m}_n] \equiv [m_{1n} m_{2n} \cdots m_{nn}] \quad (m_{1n} \geq m_{2n} \geq \cdots \geq m_{nn}) \tag{3}$$

is uniquely determined by the given irrep considered. The basis is further assumed to be lexically ordered. Thus, for the irreps $\Gamma\{2^{N/2-S}1^{2S}\}$ of $U(n)$, pertinent to N-electron model problems, we have

$$\begin{aligned} m_{in} &= 2 \quad \text{for} \quad i = 1, 2, \ldots, \tfrac{1}{2}N - S, \\ m_{in} &= 1 \quad \text{for} \quad i = \tfrac{1}{2}N - S + 1, \ldots, \tfrac{1}{2}N + S, \\ m_{in} &= 0 \quad \text{for} \quad i = \tfrac{1}{2}N + S + 1, \ldots, n; \end{aligned} \tag{4}$$

and we refer to the pertinent tableaus (1) as *electronic* Gelfand tableaus.

An equivalent canonical basis vector labeling may be achieved with Weyl tableaus,[28] which are Young tableaus in which repetitions in the same row are allowed. The pertinent Young pattern (frame), which also uniquely labels a given irrep of $U(n)$, is defined by the partition $\{2^{N/2-S}1^{2S}\}$ of N, labeling our irreps of $U(n)$. A Weyl tableau associated with a given Gelfand tableau (1) is then obtained by inserting into the ith row of the Young frame m_{ii} times number i, $(m_{i,i+1} - m_{ii})$ times number $(i+1)$, $(m_{i,i+2} - m_{i,i+1})$ times number $(i+2)$, etc, until inserting $(m_{in} - m_{i,n-1})$ times number n, for all rows $i = 1, 2, \ldots, \frac{1}{2}N + S$.

The dimension of the irreps of $U(n)$ are given by the well-known Weyl's or Robinson's formulas.

To obtain the matrix representative of the Hamiltonian, or of other observables, in the given basis one exploits the fact that any particle-number-conserving spin-independent operator may be expressed as a sum of i-degree forms in the generators E_{ij} of $U(n)$.[1] These generators satisfy the following commutation relations

$$[E_{ij}, E_{kl}]_- = \delta_{jk} E_{il} - \delta_{il} E_{kj}, \tag{5}$$

as well as the following Hermitian property

$$E_{ij}^+ = E_{ji} \tag{6}$$

for all $i, j = 1, \ldots, n$, defining fully the structure constants of the corresponding Lie algebra of $U(n)$. Thus, to obtain the desired matrix representatives of particle-number-conserving observables in the Gelfand-Tsetlin canonical basis, we only need know the representation of the pertinent Lie algebra $u(n)$ associated with $U(n)$ in this basis.

The generators E_{ij} of $U(n)$ may be classified into the lowering $(i > j)$, weight $(i = j)$, and raising $(i < j)$ generators according to whether they lower, give and raise the weight of each N-particle state, so that their representation matrices in a lexically ordered canonical basis are strictly lower triangular, diagonal, and strictly upper triangular, respectively. Further, the real representation matrices for the lowering and raising generators E_{ij} and E_{ji} $(i > j)$, respectively, are given by mutually transposed matrices as follows from (6). Finally, the raising (lowering) generator matrix representatives are fully determined by the corresponding *elementary* or *primitive*[24] generators $E_{i-1,i}$ $(E_{i,i-1})$, $(i = 2, \ldots, n)$, from which all the remaining ones may be obtained by applying the recurrence formula

$$E_{i-1,i+k} = [E_{i-1,i}, E_{i,i+k}]_-, \quad k = 1, \ldots, n-2, \tag{7}$$

which follows immediately from (5).

Explicit formulas for the matrix representatives of generators in the canonical bases were given by Gelfand and Tsetlin[3] and Baird and Biedenharn.[5] They are very simple for weight generators (occupation numbers)[29]

$$\langle [\underline{m}'] | E_{ii} | [\underline{m}] \rangle = \delta([\underline{m}], [\underline{m}'])(k_i - k_{i-1}), \tag{8}$$

where

$$k_j = \sum_{i=1}^{j} m_{ij}, \tag{9}$$

but rather complex for other generators (even the elementary ones).[3-6] It is exactly this step in the whole formalism, which may be greatly simplified[14,19,24] when we restrict our considerations to the electronic Gelfand states pertinent in the N-electron model problems.

III. N-ELECTRON FORMALISM

Restricting ourselves to an N-electron case, the entries m_{ij} of an electronic Gelfand tableau (1)–(4) may only equal 0, 1, or 2, i.e.

$$0 \leq m_{ij} \leq 2 \quad (i \leq j; \; j = 1, 2, \ldots, n). \tag{10}$$

Consequently a more economical notation is possible. For example, we can use an $n \times 3$ matrix[30] $[a_i b_i c_i]$, $(i = 1, 2, \ldots, n)$, called an ABC tableau, whose ith row integer entries a_i, b_i, and c_i give the number of 2's, 1's, and 0's in the ith row of the Gelfand tableau (1), respectively. Since, further

$$a_i + b_i + c_i = i \quad (i = 1, 2, \ldots, n), \tag{11}$$

any $n \times 2$ submatrix of an ABC tableau is sufficient: say, the AC tableau $[a_i c_i]$, $(i = 1, \ldots, n)$, containing the first and the last column of the ABC tableau. However, an ideal notation should not only enable an easy and economical storage of the necessary data, but also a simple calculus. We shall see that such a notation can be based on AC tableaus.

The lexicality (betweenness) conditions (2) immediately imply that the entries a_i and c_i ($i=1,\ldots,n$) of an AC tableau must form a finite nondecreasing sequence of integers, whose subsequent members differ at most by unity, i.e.,

$$0 \leq x_{i+1} - x_i \leq 1 \quad (x=a,c;\ i=1,\ldots,n-1). \tag{12}$$

Thus, defining the (first) difference tableau (ΔAC tableau) $[\Delta a_i \Delta c_i] \equiv [\alpha_i \gamma_i]$, ($i=1,\ldots,n$), with entries

$$\Delta x_i \equiv \xi_i = x_i - x_{i-1} \quad (x=a,\ \xi=\alpha \text{ or } x=c,\ \xi=\gamma;\ i=1,2,\ldots,n), \tag{13}$$

where for convenience we have defined

$$a_0 = b_0 = c_0 = 0, \tag{14}$$

we have that $\xi_i = 0$ or 1, so that each lexical electronic Gelfand pattern (1)–(4) may be uniquely represented by two binary strings of length n, each one consisting of one column entries of the first difference tableau.

We note that, obviously,

$$x_i = \sum_{j=1}^{i} \Delta x_j \quad (x=a,c;\ i=1,\ldots,n). \tag{15}$$

In particular, the digital sums of these binary strings [$i=n$ in (15)] must be the same for all vectors of the given irrep basis, namely

$$\begin{aligned} a &\equiv a_n = \tfrac{1}{2}N - S, \\ c &\equiv c_n = n - a - b = n - \tfrac{1}{2}N - S, \\ (b &\equiv b_n = 2S). \end{aligned} \tag{16}$$

This irrep is in turn uniquely specified by the number of electrons N, the number n of single particle states (AO's) used, and by the desired multiplicity $(2S+1)$. The dimension of this irrep $\Gamma\{2^a 1^b\}$ of $U(n)$ is[14]

$$\mathrm{Dim}(\Gamma^{U(n)}\{2^a 1^b\}) = \frac{b+1}{n+1}\binom{n+1}{a}\binom{n+1}{c}, \tag{17}$$

where $\binom{m}{n} = m!/(m-n)!n!$ is the usual binomial coefficient.

The lexicality conditions (both necessary and sufficient) for ΔAC tableaus may be expressed as follows

$$\sum_{j=i}^{n} \Delta x_j \leq x \quad (x=a,c;\ i=1,\ldots,n)$$

and (18)

$$\sum_{j=i}^{n} (\Delta a_j + \Delta c_j) > a + c - i \quad (i=1,\ldots,n).$$

Therefore, we can obtain the lexically ordered basis for a given irrep $\Gamma\{2^a 1^{n-a-c}\}$ of $U(n)$ by taking subsequently for $(\Delta a_i \Delta c_i)$, $i=n,n-1,\ldots,1$ the values (01), (00), (11), and (10), in this order, and discarding at each step the nonlexical patterns violating the lexicality conditions (18).

We next show that also the matrix representatives of weight and elementary raising (lowering) generators are simply determined in terms of the first difference tableau notation for basis vectors. For weight generators we have[29]

$$\langle [\underline{m}'] | E_{ii} | [\underline{m}] \rangle = \delta([\underline{m}'],[\underline{m}])[1 + \Delta a_i - \Delta c_i]. \tag{19}$$

The nonvanishing matrix elements of elementary raising (lowering) generators are easily determined by using the first ($k=1$) and the second ($k=2$) difference tableaus with entries

$$\Delta^k x_i = \Delta^{k-1} x_i - \Delta^{k-1} x_{i-1} \quad (x=a,c;\ k=1,2;\ i=k,k+1,\ldots,n) \tag{20}$$

where $\Delta^0 x_i \equiv x_i$. We have also designated earlier [cf., Eq. (13)] $\Delta^1 x_i \equiv \Delta x_i \equiv \xi_i$. Using this notation the entries in the $[\underline{m}]$th column of the matrix representative of an arbitrary elementary raising (and, similarly, for lowering) generator are given[14,19,24] by a simple expression

$$\langle [\underline{m}]_x^{(i)} | E_{i-1,i} | [\underline{m}] \rangle = \delta(\Delta^2 x_i, \epsilon_x)[h_i/(h_i - \Delta^2 x_i)]^{\Delta^2 a_i \Delta^2 c_i/2} \quad (x=a,c) \tag{21}$$

where

$$\epsilon_a = 1, \quad \epsilon_c = -1,$$

and

$$h_i = i - \sum_{j=1}^{i-1} (\Delta^1 a_j + \Delta^1 c_j) > \Delta^2 x_i. \tag{22}$$

The entries $\Delta^1 x_j^{(i)}$ ($j=1,\ldots,n$; $x=a,c$) of the row-determining tableau $[\underline{m}]_x^{(i)}$ are the same as those of $[\underline{m}]$ except for $j=i-1$ and $j=i$ when

$$\Delta^1 x_j^{(i)} = \delta(\Delta^1 x_j, 0) = \bar{\xi}_j = \delta(\xi_j, 0), \quad (x=a,c;\ j=i-1,i), \tag{23}$$

the bar designating the binary complementation (i.e., $\bar{1}=0; \bar{0}=1$).

Note that the exponent $\frac{1}{2}\Delta^2 a_i \Delta^2 c_i$ in (21) is either 0 or $\pm\frac{1}{2}$, so that the pertinent matrix elements equal either 1 or are given as a square root of a ratio of two integers differing by 1, respectively.[31] The parameters h_i, Eq. (22), give in fact the intermediate spin coupling quantum numbers of the Yamanouchi-Kotani genealogical basis,[32] which is up to a phase equivalent with the Gelfand-Tsetlin basis.[19] From (21) we can also conclude the following.

(i) Any row (column) of an elementary generator

matrix representative has *at most two* non-vanishing entries.

(ii) Using formula (21) we can *simultaneously* determine a given column for *all* elementary raising (lowering) generators.

(iii) The elementary generators $E_{i-1,i}$ having nonvanishing entries in the column labeled by a given ΔAC tableau $[\alpha_j \gamma_j]$, $(j=1,\ldots,n)$, are given by the row indices of the second difference tableau entries for which $\Delta^2 a_i = \Delta\alpha_i = 1$ and/or $\Delta^2 c_i = \Delta\gamma_i = -1$.

(iv) The value of the pertinent matrix element is simply determined by the parameter h_i, which in turn is simply obtained from a digital sum of the appropriate tails $(\Delta x_{i-1}\Delta x_{i-2}\ldots\Delta x_1)$, $x=a,c$, of binary strings (columns of an ΔAC tableau) labeling the column-determining N-electron state function considered [cf., Eq. (22)].

Finally, the matrix representatives of nonelementary generators (and of products of generators), may be either obtained recursively [cf., Eq. (7)] or directly.[24] Let us mention that the recursive algorithm may also be used for truncated bases, (essential for limited configuration interaction calculations[26]), when the configuration state functions are appropriately selected.[33]

Since the binary strings (arrays) may be very efficiently represented and handled on modern digital computers, we hope that the above outlined algorithms might be particularly suitable for computer implementation of the unitary group approach.

IV. RELATION TO WEYL TABLEAU FORMALISM

Harter and Patterson recently published[22] rules for the determination of matrix elements of elementary generators based on the Weyl tableau representation of N-electron spin-adapted states. We now show how their rules easily follow from our general formula (21), thus establishing the equivalence of both approaches.

The key step is to find the relationship between our first difference (ΔAC) tableau and the Weyl tableau labeling schemes. In our earlier work we have formulated[14,19,24] algorithms yielding a pertinent Weyl tableau from our ABC or AB tableaus [the latter ones being simply obtainable from AC tableaus using (11)]. Starting from this result we can in fact establish a very simple and direct relationship between our first difference (ΔAC) tableaus and the corresponding Weyl tableaus.

Consider a general Weyl tableau labeling some vector of the carrier space of the irrep $\Gamma\{2^a 1^{n-a-c}\}$ of $U(n)$, as shown in Fig. 1. Then the index families (ordered sets) I and J,

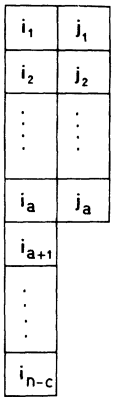

FIG. 1. General Weyl tableau for a vector of the carrier space of the irrep $\Gamma\{2^a 1^{n-a-c}\}$ of $U(n)$.

$$I \equiv \{i_1, i_2, \ldots, i_{n-c}\},$$
$$J \equiv \{j_1, j_2, \ldots, j_a\}, \tag{24}$$
$$(i_1 < i_2 < \cdots < i_{n-c};\ j_1 < j_2 < \cdots < j_a)$$

labeling the columns and, thus, uniquely defining a given Weyl tableau are determined by the first difference (ΔAC) tableau entries as follows:

$$i \in I \Leftrightarrow \Delta c_i = 0$$
$$i \notin I \Leftrightarrow \Delta c_i = 1 \tag{25}$$

and

$$i \in J \Leftrightarrow \Delta a_i = 1$$
$$i \notin J \Leftrightarrow \Delta a_i = 0.$$

Thus, by writing the row indices of the unit (vanishing) entries of the first (second) column of a given ΔAC tableau into the second (first) column of the pertinent Young frame, we immediately obtain the corresponding Weyl tableau as the example in Fig. 2 of a vector in the basis for the irrep $\Gamma\{2^2 1^2\}$ of $U(6)$ illustrates.

It is now easy to obtain Harter and Patterson's rules (cf., Fig. 3 of Ref. 22) for the different cases they distinguish. Consider, for example, the case with doubly occupied orbital (i) and unoccupied orbital ($i-1$) [i.e., the second case (c) and the first case (d) of Harter and Patterson[22]], characterized by the Weyl tableau shown schematically in Fig. 3 [only labels (i) and ($i-1$) are shown explicitly], where v and u give the number of nodes (boxes) in the first and the second columns preceding the node labeled (i).

Clearly, this situation corresponds to the following structure of the ith and $(i-1)$th rows of our ΔAC tableau

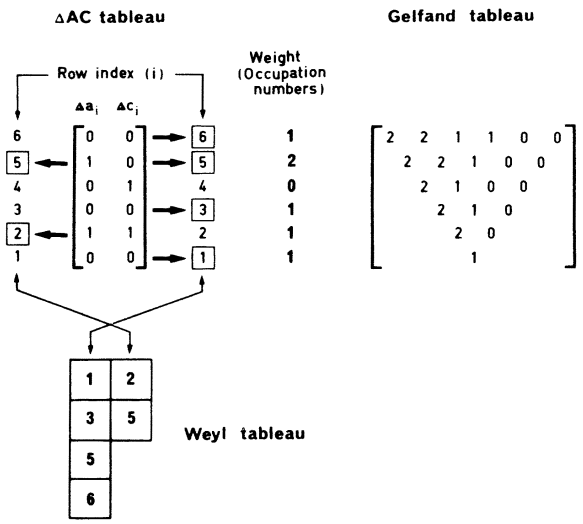

FIG. 2. An illustration of the relationship between ΔAC, Gelfand, and Weyl tableaus representing the same vector in the basis for the irrep $\Gamma\{2^2 1^2\}$ of $U(6)$.

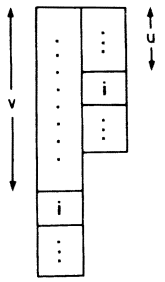

FIG. 3. Weyl tableau characterizing the case with doubly occupied orbital (i) and unoccupied orbital $(i-1)$.

Row index (j)	Δa_j	Δc_j	Occupation number	
$j=i$	1	0	2	(26)
$j=i-1$	0	1	0	

Since $\Delta^2 a_i = 1$ and $\Delta^2 c_i = -1$ neither matrix element given by (21) vanishes and we get

$$\langle [\underline{m}]_a^{(i)} | E_{i-1,i} | [\underline{m}] \rangle = [(h_i - 1)/h_i]^{1/2} \tag{27a}$$

and

$$\langle [\underline{m}]_c^{(i)} | E_{i-1,i} | [\underline{m}] \rangle = [(h_i + 1)/h_i]^{1/2}, \tag{27b}$$

where h_i is given by (22). Recalling the relationship between the ΔAC and Weyl tableaus given above, we find immediately that u and v are given by the number of unit and zero entries in the rows $j = 1, 2, \ldots, (i-1)$ of the first and second column of the corresponding ΔAC tableau, respectively, so that

$$u = \sum_{j=1}^{i-1} \Delta a_j$$

and (28)

$$v = (i-1) - \sum_{j=1}^{i-1} \Delta c_j .$$

Consequently

$$h_i = v - u + 1 \equiv d \tag{29}$$

may be interpreted as a "city block" distance[22] between labels (i) in the first and second columns of the Weyl tableau shown in Fig. 3.

Furthermore, using (23) we see immediately that the left-hand side patterns in (27a) and (27b) are simply obtained by replacing (i) by $(i-1)$ in the second and first columns of the Weyl tableau shown in Fig. 3, respectively.

In exactly the same way, we can obtain the rules for the cases when both (i) and $(i-1)$ are singly occupied, corresponding to the first case (c) and the second case (d) of Harter and Patterson.[22] We find that the "city block" distance d equals $(h_i - 1)$ and $(h_i + 1)$ in the first and the second cases mentioned, respectively. Finally, by considering the remaining cases when (i) is singly occupied and $(i-1)$ is either unoccupied or doubly occupied, i.e., cases (g) and (h) of Harter and Patterson,[22] we find immediately that always $\Delta^2 a_i \, \Delta^2 c_i = 0$, so that the pertinent matrix elements equal 1.

Concluding this comparison let us note that we can also easily reformulate Harter and Patterson's[22] "assembly formulas" in terms of our ΔAC tableaus: we simply proceed from the top of the ΔAC tableau, while the quantities μ_1 and μ_2 are given by the number of remaining 0's and 1's in the second and the first column, respectively.

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[26]For a recent extensive review see I. Shavitt, in *Modern Theoretical Chemistry, Vol. 2, Electronic Structure: Ab Initio Methods*, edited by H. F. Schaefer, III (Plenum, New York, to be published).

[27]This clearly includes so called *"ab initio"* calculations, where the model Hamiltonian is defined by the chosen (finite!) one-electron basis.

[28]It should be noted that Weyl bases are not identical (or even simply related) with Gelfand-Tsetlin canonical bases [except in the simplest case of SU(2)], the former ones being not even orthogonal in the general case. However, there is a simple one-to-one correspondence between both Weyl and Gelfand labeling schemes, which may be effectively used in either case (cf., for example, Ref. 6).

[29]For typographical reasons we write the Kronecker delta as follows: $\delta(i,j) \equiv \delta_{ij}$. Further, $\delta([\underline{m}],[\underline{m}'])$ clearly means

$$\delta([\underline{m}],[\underline{m}']) = \prod_{i \le j=1}^{n} \delta(m'_{ij}, m_{ij}) .$$

[30]We use systematically the reversed row ordering as in the Gelfand tableau (1); i.e., we label the rows in our $n \times 3$ or $n \times 2$ matrices from the bottom row ($i = 1$) to the top row ($i = n$). As a reminder of this convention we use the term tableau for these matrices.

[31]This fact may in turn be exploited for an efficient storage of these matrix elements.

[32]This fact may enable one to establish the relationship of our approach with that of Gouyet *et al.*[17] However, these authors give formulas for the generators E_{in} ($i < n$).

[33]J. Paldus, unpublished results.