The Combinatorics of Graphical Unitary Group Approach to Many Electron Correlation

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The combinatorics of Gel'fand states which are useful in the graphical unitary group approach to many electron correlation problem and spin free quantum chemistry is considered. Using operator theoretic methods it is shown that the generators of Gel'fand states are S-functions.

Key words: Gel'fand states, combinatorics of $\sim$ – S-functions – Graphical unitary group, combinatorics of $\sim$.

1. Introduction

In recent years graph theory and combinatorics have been shown to have several potentially useful chemical applications. For a review of this topic see the book of Balaban [1]. The graphical unitary group approach to many electron correlation problem developed by Paldus and expounded by several others is one such application [2–10]. This approach essentially speeds up the evaluation of the symbolic formulas for CI Hamiltonian matrix elements. It is well known that the basis sets for the unitary groups can be described by the Gel'fand–Tsetlin bases or the associated Gel'fand tableau or Weyl tableau. One of the objectives of this paper would be to describe the combinatorics of the enumeration of Gel'fand states by the way of the appropriate generating function techniques. Using operator theoretic methods it is shown that the generators of Gel'fand states are Schur functions.

Gel'fand states have been independently described and used by Matsen [11] in spin free quantum chemistry. Most of these problems involve or require the enumeration of Gel'fand states. The usual genealogical construction of spin

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functions [12] can be achieved using Gel'fand states. Further, using the representation theory of generalized wreath products developed by the author [13] and operator theoretic methods [14], it is possible to compose S-functions to what we call generalized plethysms which are generalizations of plethysms outlined in Read's [15] paper. When such generalizations have been accomplished with the group theoretical concepts developed by the author [16] in NMR spectroscopy, it would be possible to elegantly generate NMR spin functions. More over, these generalized plethysms will have applications in the enumeration of non-rigid isomers and NMR signals, the essential basic foundations of which have been laid in the papers [17–19]. This paper uses operator theoretic formulations of Williamson [20] for abelian characters which have been recently generalized to nonabelian characters by Merris [21]. Some of the elementary concepts used in this paper can be found in the books [22–24] and the paper of Knuth [25]. A correspondence between Gel'fand states and the irreducible representations of the symmetric groups can be found in the paper of Moshinsky [26]. In an earlier paper the author [27] introduced operator methods and combinatorics in symmetry adaptation. Sect. 2 describes the preliminaries and definitions, Sect. 3 discusses imminants, S-functions and group characters; in Sect. 4 we give operator theoretic formulations and Sect. 5 concludes with the generation of Gel'fand states.

2. Definitions and Preliminaries

2.1. Partitions, Gel'fand States, Gel'fand–Tsetlin Tableau

An m-tuple $(\alpha_1, \alpha_2, \ldots, \alpha_m)$ satisfying

$$n = \alpha_1 + \alpha_2 + \cdots + \alpha_m, \alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_m \geq 1$$

is called a partition of an integer n into m parts. With any partition of an integer we can associate a diagram in which the ith component of the m-tuple defined above is represented by the ith row containing α_i squares. For example, Fig. 1 shows the diagram (known as Young's diagram) associated with the partition $(3, 1, 1)$. (In Fig. 1, squares are filled with certain integers and their significance can be seen in the ensuing discussion). The number of partitions of an integer n into m parts is denoted as P_n^m and the total number of partitions of n is P_n. The generating functions for P_n and P_n^m are given by the expressions 1 and 2.

$$GF_1 = (1-x)^{-1}(1-x^2)^{-1}(1-x^3)^{-1} \cdots \tag{1}$$

$$GF_2 = x^m (1-x)^{-1}(1-x^2)^{-1} \cdots (1-x^m)^{-1}. \tag{2}$$

The coefficients of x^n in (1) and (2), give P_n and P_n^m, respectively. For a proof, see Berge [23]. With every partition α we can associate a conjugate partition $\alpha^* = (\alpha_1^*, \alpha_2^*, \ldots, \alpha_m^*)$ which is obtained by rotating the Young's diagram of α
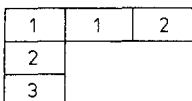
Fig. 1. A generalized Young tableau of the type $[1^2 2^2 3]$ which corresponds to the partition $3 + 1 + 1$

$$
\begin{array}{ccc}
1 & 2 & 3 \\
4 & 5 & \\
6 & &
\end{array}
$$

Fig. 2. A standard tableau associated with the partition $3 + 2 + 1$

about the diagonal. For example, the conjugate of the partition $3 + 2 + 1 + 1$ is $4 + 2 + 1$. Given a partition of the integer n we can associate a standard tableau by filling each square with integers $1, 2, \ldots, n$ such that the integers are strictly in increasing order from left to right and top to bottom. For example, a standard tableau associated with the partition $3 + 2 + 1$ is shown in Fig. 2.

A square tableau $((h_j^i))$ also known as hook graph, associated with a partition is defined by

$$
h_j^i = 1 + (\alpha_i - j) + (\alpha_j^* - i). \tag{3}
$$

For example, the square tableau associated with the partition $3 + 2 + 1$ is shown in Fig. 3.

$$
\begin{array}{ccc}
5 & 3 & 1 \\
3 & 1 & \\
1 & &
\end{array}
$$

Fig. 3. The square tableau or the hook graph associated with the partition $3 + 2 + 1$

Frame, Robinson and Thrall [29] proved an important theorem which relates the number of standard tableaus associated with a partition and the square tableau associated with this partition. In fact, according to this theorem, the number of standard tableaus $N(\alpha_1, \ldots, \alpha_m)$, is given by

$$
N(\alpha_1, \alpha_2, \ldots, \alpha_m) = n! \bigg/ \prod_{i,j} h_j^i.
$$

There is a correspondence between the theory of partitions and the representation theory of the symmetric groups. With every irreducible representation of S_n we can associate a partition of the integer n and there are exactly P_n irreducible representations in S_n. The dimension of an irreducible representation is the number of standard tableaus that can be constructed with the associated partition. The characters of the irreducible representations of S_n are obtainable using the diagrams associated with the partition. For a review of this topic, see Hamermesh [28].

A generalized Young tableau also known as Weyl tableau is defined as a tableau containing integers chosen from the set $\{1, 2, \ldots, n\}$ such that integers are in nondecreasing order in any row and they are in strictly increasing order in any column. For example, a generalized Young tableau is shown in Fig. 1. A generalized Young tableau (GYT) containing λ_1 integers of the type α_1, λ_2 integers of the type $\alpha_2, \ldots, \lambda_t$ integers of the type α_t can be denoted as $[\alpha_1^{\lambda_1} \alpha_2^{\lambda_2} \cdots \alpha_t^{\lambda_t}]$. There are many ways one can form GYT's. For example, all GYT's of the type $[1^2 2^2 3^2]$ are shown in Fig. 4.
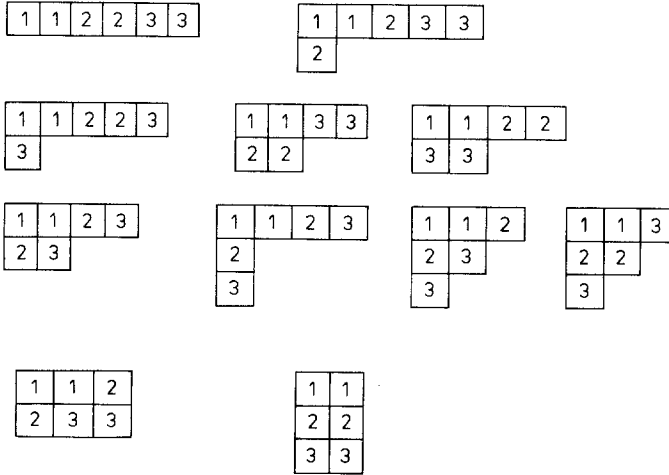
Fig. 4. All generalized Young tableaus of the shape $[1^2 2^2 3^2]$ which correspond to the partitions of the integer 6

The basis vectors of the irreducible representations of $U(n)$ can be uniquely labeled by a triangular pattern defined by Gel'fand known as a Gel'fand–Tsetlin tableau shown below.

$$[m] = \begin{bmatrix} m_n \\ m_{n-1} \\ \vdots \\ m_2 \\ m_1 \end{bmatrix} = \begin{bmatrix} m_{1n} & m_{2n} & \cdots & m_{n-1,n} & m_{nn} \\ & m_{1,n-1} & \cdots & m_{n-1,n-1} & \\ & & \vdots & & \\ & m_{12} & & m_{22} & \\ & & m_{11} & & \end{bmatrix}$$

The integers in this triangular array satisfy the following condition:

$$m_{i,j} \geq m_i, \qquad j-1 \geq m_{i+1,j},$$

for all $i = j, \ldots, n-1, j = 2, 3, \cdots, n$.

There is a one-to-one correspondence between a Gel'fand–Tsetlin tableau and a GYT of appropriate shape. The first row of the given Gel'fand–Tsetlin tableau determines the Young diagram. Then one fills integers from the set $\{1, 2, \ldots, n\}$ such that in the ith row of the diagram, i is filled in the first m_{ii} boxes, $i+1$ in the next $m_{i,i+1} - m_{ii}$ boxes etc., until n is filled in the last $m_{in} - m_{i,n-1}$ boxes.

The GYT's pertaining to N-electron problem can contain at most two columns because of the Pauli principle. Paldus calls the Gel'fand–Tsetlin tableaus associated with electron problems the electronic tableaus. The associated *ABC* tableaus introduced by Paldus as a short hand notation for electronic Gel'fand tableaus are called Paldus tableaus. Thus, the Gel'fand–Tsetlin tableau is characterized by a $n \times 3$ matrix which gives the number of 2's, 1's and zeros in a given row of Gel'fand tableaus. In fact, in this case the corresponding GYT's can be

characterized by α-β tableaus which are obtained by generating GYT's with α's and β's with a lexical ordering $\beta > \alpha$. That is, in any row α's and β's occur in non-decreasing order and in any column α's and β's occur in strictly increasing order. Consequently, there can be at most 2 rows. The labels α and β can be associated with the spin up and spin down of the electron, respectively.

2.2. Cycle Indices, Patterns and Generating Functions

Let G be a group acting on a discrete set D. Let F denote the set of all maps from the set D to another discrete set R. G also acts on F in that if $f \in F$ then

$$g(f(i)) = f(g^{-1}i) \quad \text{for every } i \in D.$$

Define the cycle index of G to be

$$P_G = \frac{1}{|G|} \sum_{g \in G} x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n}$$

where $x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n}$ is a representation of a typical permutation $g \in G$ which has b_1 cycles of length 1, b_2 cycles of length 2, etc.

Two maps $f_1, f_2 \in F$ are said to be G-equivalent if there exists a $g \in G$ such that

$$f_1(d) = f_2(gd) \quad \text{for every } d \in D.$$

All equivalent maps form a G-equivalence class which is called a pattern. Thus G acts on F and divides F into patterns.

Let w be a function $w: R \to K$, where K is a field of characteristic zero. Then for each $f \in F$ we can define a map $W: F \to K$ which is also a constant on the orbits resulting from the action of G on F as follows:

$$W(f) = \prod_{i=1}^{d} w(f(i)).$$

Pólya [30] showed that the configuration counting series which is a generating function for patterns is obtained by the following substitution in the cycle index:

$$\text{G.F.} = P_G\left(x_k \to \sum_{r \in R} w^k(r)\right).$$

Coefficient of a typical term $w^{b_1}(r_1)w^{b_2}(r_2) \cdots$ gives the number of patterns with the weight $w^{b_1}(r_1)w^{b_2}(r_2) \cdots$.

3. Imminants, S-Functions and Group Characters

Let $[a_{ij}]$ be a matrix of order $n \times n$. Let s be a permutation belonging to the group S_n of the type $e_1, e_2, \ldots, e_n$ of the numbers $1, 2, \ldots, n$. Let P_s be the product

$$P_s = a_{1e_1} a_{2e_2} \cdots a_{ne_n}.$$

Let $\chi^{(\lambda)}$ be the character associated with the irreducible representation $[\lambda]$ of S_n corresponding to the partition $(\lambda) = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ of n. Then the imminant of the matrix $[a_{ij}]$ which corresponds to the partition (λ) is given by

$$|a_{ij}|^{(\lambda)} = \sum \chi^{(\lambda)}(s) P_s$$

where the sum is taken over all $n!$ permutations of S_n. Note that for $(\lambda) = (n, 0, 0, \ldots, 0)$, $|a_{ij}|^{(\lambda)}$ is the symmetrizer and for $(\lambda) = (1, 1, 1, \ldots, 1)$, $|a_{ij}|^{(\lambda)}$ is the antisymmetrizer.

Consider a symmetric function s_r of the quantities $\alpha_1, \alpha_2, \ldots, \alpha_n$, defined by

$$s_r = \sum_{i=1}^{n} \alpha_i^r.$$

Let Z_r be the matrix defined by

$$[Z_r] = \begin{bmatrix} s_1 & 1 & 0 & 0 & & \cdots & & 0 \\ s_2 & s_1 & 2 & 0 & & \cdots & & 0 \\ s_3 & s_2 & s_1 & 3 & 0 & \cdots & & 0 \\ \vdots & & & & & & & \\ s_{r-1} & s_{r-2} & & \cdots & & & s_1 & r-1 \\ s_r & s_{r-1} & & \cdots & & & s_2 & s_1 \end{bmatrix}$$

If (λ) is a partition $(\lambda) \equiv (\lambda_1, \lambda_2, \ldots, \lambda_p)$ of r with p components in descending order then the Schur function also known as S-function $\{\lambda\} = \{\lambda_1, \lambda_2, \ldots, \lambda_p\}$ is defined by the following expression:

$$\{\lambda\} = \frac{1}{r!} |Z_r|^{(\lambda)}$$

where $|Z_r|^{(\lambda)}$ is the imminant of the matrix Z_r associated with the partition (λ). Let h_r and a_r denote the S-functions which correspond to the partitions (r) and (1^r), respectively. It can be shown that the above expression for the S-function $\{\lambda\}$ can be reduced to another convenient form. Let $|C|$ be the order of conjugacy class C of the group S_n and let $\chi_C^{(\lambda)}$ be the character of $[\lambda]$ which corresponds to the class C. Then it can be shown that

$$\{\lambda\} = \frac{1}{r!} \sum_C |C| \chi_C^{(\lambda)} s_C$$

where s_C is defined by

$$s_C = s_1^{b_1} s_2^{b_2} s_3^{b_3} \cdots$$

if the conjugary class C has the cycle representation of b_1 cycles of length 1, b_2 cycles of length 2, etc. $|C|$ can be obtained by Cayley's counting principle as

$$|C| = \frac{r!}{1^{b_1} b_1! 2^{b_2} b_2! \ldots}.$$

Let us illustrate S-functions with examples from the group S_3. The symmetric group S_3 has three irreducible representations associated with partitions (3), (2, 1) and (1^3). From the character table of S_3 it can be seen that

$$\{3\} = \tfrac{1}{6}(s_1^3 + 3s_1 s_2 + 2s_3)$$

$$\{2, 1\} = \tfrac{1}{6}(2s_1^3 - 2s_3)$$

$$\{1^3\} = \tfrac{1}{6}(s_1^3 - 3s_1 s_2 + 2s_3)$$

with

$$s_k = (\alpha_1^k + \alpha_2^k + \alpha_3^k).$$

S-functions can be obtained as quotient of determinants using the Frobenius' formula which we shall briefly discuss. Let

$$\Delta(\alpha_1, \alpha_2, \ldots, \alpha_m) = \prod (\alpha_r - \alpha_s)(r < s) = \sum \pm \alpha_1^{m-1} \alpha_2^{m-2} \cdots \alpha_{m-1}.$$

Then the Frobenius formula which relates s_C, $\Delta(\alpha_1, \ldots, \alpha_n)$ and the character is shown below.

$$s_C \Delta(\alpha_1, \alpha_2, \ldots, \alpha_m) = \sum \pm \chi_C^{(\lambda)} \alpha_1^{\lambda_1 + n - 1} \alpha_2^{\lambda_2 + n - 2} \cdots \alpha_n^{\lambda_n}.$$

From this it can be easily shown that

$$\{\lambda\} = \frac{1}{r!} \sum |C| \chi_C^{(\lambda)} s_C = \frac{\sum \pm \prod_i \alpha_i^{\lambda_i + n - i}}{\sum \pm \prod_i \alpha_i^{n - i}}$$

where

$$|C| = \frac{r!}{1^{b_1} b_1! 2^{b_2} b_2! \ldots}$$

if the conjugacy class C contains b_1 cycles of length 1, b_2 cycles of length 2, ..., etc. The summation is taken with respect to all permutations, the negative sign is for odd permutations.

Generating functions can be obtained for S-functions as follows. Let $F(x) = 1 + \sum h_r x^r$ where h_r is the S-function which corresponds to the partition (r). Consider the S-function of the form $\{n, p_1, p_2, \ldots, p_i\}$ with $n \geq p_1 \geq p_2 \geq \cdots \geq p_i$. Let $g(x)$ be defined as follows:

$$g(x) = \begin{vmatrix} x^i & x^{i-1} & \cdots & 1 \\ h_{p_1 - 1} & h_{p_1} & \cdots & h_{p_1 + i - 1} \\ h_{p_2 - 2} & h_{p_2 - 1} & \cdots & h_{p_2 + i - 2} \\ \vdots & \vdots & & \vdots \\ h_{p_i - i} & h_{p_i - i + 1} & \cdots & h_{p_i} \end{vmatrix}.$$

Then $F(x)g(x)$ is a generating function for S-functions of the form $\{n, p_1, p_2, \ldots, p_i\}$. The coefficient of x^{n+i} in $F(x)g(x)$ gives $\{n, p_1, p_2, \ldots, p_i\}$.

The above methods of generating the S-functions amount to using the cycle indices of smaller groups. Let P_{S_i} be the cycle index of the symmetric group S_i. Then the S-function $\{n; p_1, p_2 \cdots p_n\}$ is precisely the determinant, det $(P_{S_{(p_i-i+j)}})$, with the convention $P_{S_0} = 1$ and $P_{S_{-l}} = 0$ for a positive integer l [31]. Let us illustrate this with the S-function $\{6; 4, 1, 1\}$. This is shown below as a determinant

$$\{6; 4, 1, 1\} = \begin{vmatrix} P_{S_4} & P_{S_5} & P_{S_6} \\ P_{S_0} & P_{S_1} & P_{S_2} \\ 0 & P_{S_0} & P_{S_1} \end{vmatrix}$$

$$= P_{S_1}^2 P_{S_4} - P_{S_2} P_{S_4} - P_{S_1} P_{S_5} + P_{S_6}$$

$$P_{S_1} = s_1$$

$$P_{S_2} = \tfrac{1}{2}(s_1^2 + s_2)$$

$$P_{S_4} = \tfrac{1}{24}(s_1^4 + 6s_1^2 s_2 + 8s_1 s_3 + 3s_2^2 + 6s_4)$$

$$P_{S_5} = \tfrac{1}{120}(s_1^5 + 10s_1^3 s_2 + 20s_1^2 s_3 + 15s_1 s_2^2 + 30s_1 s_4$$
$$+ 20s_2 s_3 + 24s_5)$$

$$P_{S_6} = \tfrac{1}{720}(s_1^6 + 15s_1^4 s_2 + 40s_1^3 s_3 + 45s_1^2 s_2^2 + 90s_1^2 s_4$$
$$+ 120s_1 s_2 s_3 + 144s_1 s_5 + 15s_2^3 + 90s_2 s_4$$
$$+ 40s_3^2 + 120s_6).$$

Substituting these expressions in the determinant expansion we find that

$$\{6; 4, 1, 1\} = \tfrac{1}{720}(10s_1^6 + 30s_1^4 s_2 + 40s_1^3 s_3 - 90s_1^2 s_2^2$$
$$- 120s_1 s_2 s_3 - 30s_2^3 + 40s_3^2 + 120s_6).$$

4. Operator Theoretic Formulations

With G, D, R and F as defined in Sect. 2.2, let us generalize the formulations in Sects. 2 and 3 by operator theoretic methods. Let V be a vector space of dimension $|R|$ over the field K. Let V^d denote $\bigotimes^d V$, the dth tensor product of V. $d = |D|$. Let $e_1, e_2, \ldots, e_{|R|}$ be a basis for V. To each $f \in F$, we can assign an

$$e_f = e_{f(1)} \otimes e_{f(2)} \otimes \cdots \otimes e_{f(d)},$$

which is a tensor. The set of tensors $S = \{e_f : f \in F\}$ forms a basis for the tensor product V^d. Define for any $g \in G$, $P(g)e_f = e_{gf}$. Thus $P(g)$ is a permutation operator relative to the basis S since it permutes the tensors in S by way of the action of g on the functions. Let $\chi : G \to K$ be a character of G. Even though this operator theoretic formulation was developed by Williamson for characters of unit degree, this was extended by Merris [21] to characters of higher degrees. Define an operator T_G^χ which we shall call a symmetry operator as follows:

$$T_G^\chi = \frac{1}{|G|} \sum_{g \in G} \chi(g) P(g).$$

Let us consider the subspace V_x^d of V^d spanned by all tensors $S_x = \{e_f: W(f) = x \in K\}$ where $W(f)$ is defined in Sect. 2.2. Let the restrictions of the operators T_G^χ and $P(g)$ to the space V_x^d be $T_G^{x,\chi}$ and $P_x(g)$, respectively. Thus one can define a weighted permutation operator with the weight W, denoted as $P_W(g)$, and a weighted symmetry operator with the weight W denoted as $T_G^{W,\chi}$ by

$$P_W(g) = \bigoplus_{x \in K} x P_x(g)$$

$$T_G^{W,\chi} = \bigoplus_{x \in K} x T_G^{x,\chi}$$

where $\bigoplus$ denotes finite direct sum with respect to the associated subspaces V_x^d and x's vary over the elements of F. It can be seen that if one considers a matrix representation of $P_W(g)$ then

$$\text{tr } P_W(g) = \sum_f^{(g)} W(f)$$

where the sum is taken over all f for which $gf = f$ and tr denotes the trace of the operator. In this set up Williamson and Merris proved the following theorem for characters of unit degree and higher degrees, respectively.

Theorem 1:

$$T_G^{W,\chi} = \frac{1}{|G|} \sum_{g \in G} \chi(g) P_W(g).$$

Thus

$$\text{tr } T_G^{W,\chi} = \frac{1}{|G|} \sum_{g \in G} \chi(g) \text{ tr } (P_W(g))$$

$$= \frac{1}{|G|} \sum_{g \in g} \chi(g) \sum_f^{(g)} W(f).$$

We now extend the concept of the cycle index of a group defined in Sect. 2.2 to the cycle index of a group with character χ as

$$P_G^\chi = \frac{1}{|G|} \sum_{g \in G} \chi(g) x_1^{b_1} x_2^{b_2} \cdots$$

where $x_1^{b_1} x_2^{b_2} \cdots$ has the same meaning as in the usual cycle index. Then it can be shown by theorem 1 that

$$\text{tr } T_G^{W,\chi} = P_G^\chi \left(x_k \to \sum_{r \in R} w^k(r) \right).$$

$\text{tr } T_G^{W,\chi}$ is a generating function for patterns if χ is the character of the identity representation since each pattern contains exactly one identity representation. Each pattern which is a G-equivalence class of F contains the set of functions which are equivalent under the action of G. Thus each pattern transforms in general as a reducible representation of G which can be broken down into a direct

sum of irreducible representations. tr $T_G^{W,\chi}$ with character χ is a generating function for the irreducible representation whose character is χ contained in the pattern with the appropriate weight.

5. Generating Functions for Gel'fand States

In general, for an n-particle problem the symmetric group is S_n. Consider D as the set of these n particles and R as the possible spin states. Then each spin configuration of n-particles can be considered as a map from D to R. The group S_n divides the set of all maps from D to R into patterns. Each pattern contains exactly one identity representation of S_n. The spin configurations contained in each pattern form a reducible representation of S_n which decomposes into irreducible representations of S_n. These irreducible representations are precisely the generalized Young tableau or Gel'fand states formed by the possible spin states of the particles. This can be seen from the correspondence of unitary groups and symmetric groups. Consequently, Gel'fand states contained in each pattern can be generated by the operator theoretic formulation outlined in Sect. 4.

Let G be the symmetric group S_n. Let $w(r)$'s be the weights of spin states in the set R. Then tr $T_G^{W,\chi}$, with $T_G^{W,\chi}$ defined as in Sect. 4 with the character χ generates the Gel'fand states formed by the spin states with the Young diagram associated with the irreducible representation whose character is χ. With $G = S_n$, χ being the character associated with the irreducible representation $[\lambda]$ where λ is the partition $(\lambda_1, \lambda_2, \ldots, \lambda_p)$ it can be seen that tr T_G^W is the S-function $\{\lambda\}$. This indeed independently verifies that S-functions defined in Sect. 3 are the generating functions of the Gel'fand states.

Let us illustrate with examples. Consider a 3-particle problem which exhibits 3 spin states whose weights are α_1, α_2 and α_3, respectively. Let us find the Gel'fand states associated with these spin states and the irreducible representation $[2, 1]$ of S_3.

$$P_G^{[2,1]} = \tfrac{1}{6}[2x_1^3 - 2x_3]$$

$$\text{tr } T_G^{W,[2,1]} = \{\alpha_1\alpha_2\alpha_3; : \cdot\} = \tfrac{1}{6}[2(\alpha_1 + \alpha_2 + \alpha_3)^3 - 2(\alpha_1^3 + \alpha_2^3 + \alpha_3^3)]$$

$$= \alpha_1^2\alpha_2 + \alpha_1\alpha_2^2 + \alpha_2\alpha_3^2 + \alpha_2^2\alpha_3 + \alpha_1\alpha_3^2 + \alpha_1^2\alpha_3 + 2\alpha_1\alpha_2\alpha_3.$$

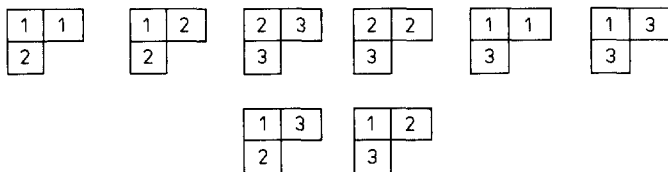The Gel'fand states thus generated are shown in Fig. 5.

Fig. 5. The possible Gel'fand states of a particle possessing 3 spin states which correspond to the partition (2, 1)

Another nontrivial example which illustrates the generation of Gel'fand states would be the Gel'fand states associated with 4 particles with 3 spin states corresponding to the partition (3, 1).

$$P_G^{[3,1]} = \tfrac{1}{24}[3x_1^4 + 6x_1^2x_2 - 6x_4 - 3x_2^2]$$

$$\text{tr } T_G^{W,[2,1]} = \{\alpha_1\alpha_2\alpha_3; : \cdot \cdot\}$$

$$= \tfrac{1}{24}[3(\alpha_1 + \alpha_2 + \alpha_3)^4 + 6(\alpha_1 + \alpha_2 + \alpha_3)^2(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)$$

$$-6(\alpha_1^4 + \alpha_2^4 + \alpha_3^4) - 3(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)^2].$$

This on simplification yields

$$\alpha_1^3\alpha_2 + \alpha_1^3\alpha_3 + \alpha_1\alpha_2^3 + \alpha_2^3\alpha_3 + \alpha_1\alpha_3^3 + \alpha_2\alpha_3^3 + \alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_3^2$$

$$+\alpha_2^2\alpha_3^2 + 2\alpha_1^2\alpha_2\alpha_3 + 2\alpha_1\alpha_2^2\alpha_3 + 2\alpha_1\alpha_2\alpha_3^2.$$

The total number of tableaus can also be obtained by replacing every x_k by $|R|$ in the cycle index of G with the appropriate character. In this case it is

$$\tfrac{1}{24}[3 \cdot 3^4 + 6 \cdot 3^2 \cdot 3 - 6 \cdot 3 - 3 \cdot 3^2] = 15.$$

The Gel'fand states thus generated are shown in Fig. 6. The Gel'fand states shown in Figs. 4, 5 and 6 can also be obtained by the canonical basis set procedure (see Paldus [5]). The total number of all possible Gel'fand states associated with a partition of n and the symbols $\alpha_1, \alpha_2, \ldots, \alpha_n$ can be obtained by the following formula described by Matsen [32].
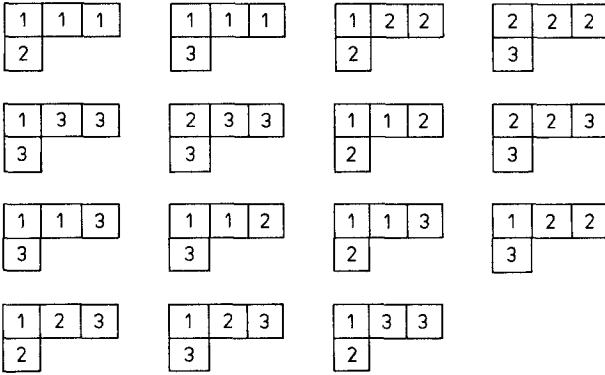
$$N(\alpha_1, \alpha_2, \ldots, \alpha_n; p_1, p_2, \ldots) = \frac{\prod n^{(p_1 p_2, \ldots)}}{\prod\limits_{i,j} h_j^i}$$

where

$$n^{(p_1, p_2, \ldots)} = \begin{array}{|c|c|c|}\hline n & n+1 & n+2 \\ \hline\end{array} \cdots$$

$$\begin{array}{|c|c|}\hline n-1 & n \\ \hline\end{array} \cdots$$

$$\begin{array}{|c|c|}\hline n-2 & n-1 \\ \hline\end{array} \cdots$$

$$\begin{array}{|c|}\hline n-3 \\ \hline\end{array} \cdots$$

$$\vdots$$

For the example [2, 1] in S_3 the total number of Gel'fand states as obtained by this formula, is

$$N(\alpha_1, \alpha_2, \alpha_3; 2, 1) = \frac{3 \cdot 4 \cdot 2}{3} = 8.$$

Fig. 6. The 15 Gel'fand states of a particle possessing 3 spin states which correspond to the partition (3, 1)

However, this method can give only the total number of Gel'fand states associated with a partition containing the symbols chosen from the set $\{\alpha_1, \alpha_2, \ldots, \alpha_n\}$.

For an electron problem the set R has only two elements since electrons are characterized by just two spin states, namely α and β. The appropriate Gel'fand states are thus generalized Young tableaus formed by 1's and 2's only. If we associate a weight α_1 to the spin state α and a weight α_2 to the spin state β, then all the S-functions of the type $\{\alpha_1\alpha_2; \lambda\}$ where (λ) is the set of all partitions of the integer n generate the corresponding Gel'fand states. However, the Pauli principle restricts (λ) to contain at most two components and hence $(\lambda) = (\lambda_1, \lambda_2)$ for an n-electron problem. Each pattern of spin configurations splits into irreducible representations which are sums of Young diagrams associated with the Gel'fand
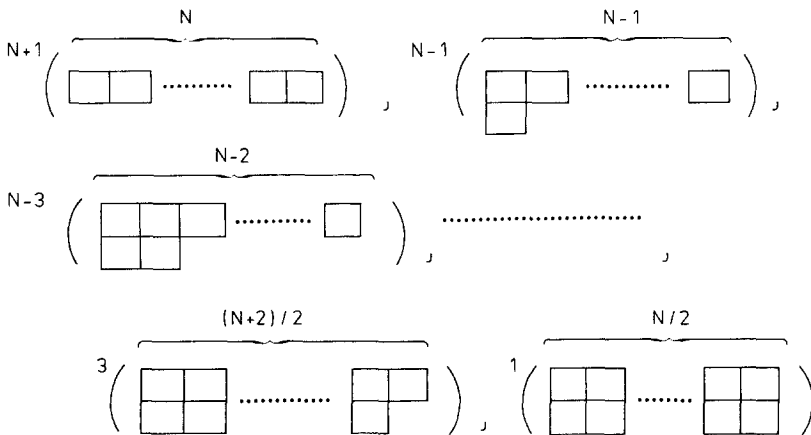
Fig. 7. The multiplets of spin species of N electrons for even N. The Young diagram specifies the irreducible representation of the corresponding spin species
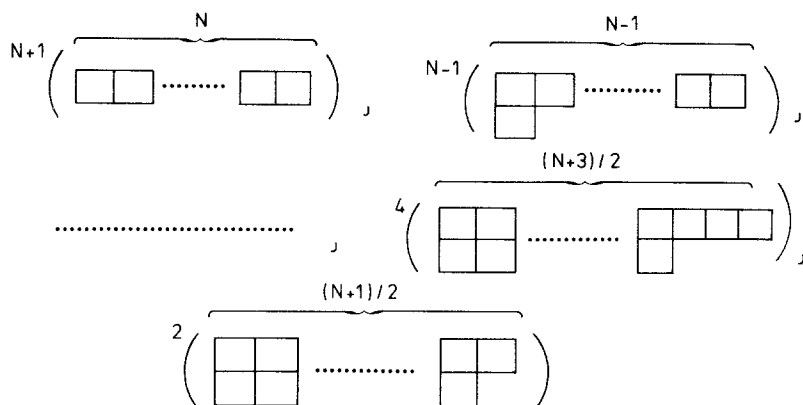
Fig. 8. The multiplets of spin species of electrons for odd N

states of appropriate weight. For example, the spin pattern $\alpha\alpha\alpha\alpha\beta$ for a 6-electron problem splits into $\underset{\beta}{\alpha\alpha\alpha\alpha} \oplus \alpha\alpha\alpha\alpha\beta$.

A class with the weight $\alpha_1^{b_1}\alpha_2^{b_2}$ corresponds to spin $(b_1 - b_2)/2$. Consequently, when one groups Young diagrams with various spins they form a triangular array. If there are N electrons then all spin states can be generated this way and they are shown in Figs. 7 and 8 for even and odd numbers of electrons, respectively. The Young diagram specifies the spin species.

Recently, the author [33] introduced operator methods in molecular spectroscopy for developing a method for nuclear spin statistics.

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