Symmetric Functions and the Symmetric Group 5

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To do research you don't have to know everything
All you have to know is one thing that is not known
–Art Schawlow *Nobel Laureate*

5.1 $S-$function series

Infinite series of $S-$functions play an important role in determining branching rules and furthermore lead to concise symbolic methods well adapted to computer implementation. Consider the infinite series

$$\begin{aligned} L &= \prod_{i=1}^{\infty}(1-x_i) \\ &= 1 - \sum x_1 + \sum x_1x_2 - \ldots \end{aligned} \tag{5.1}$$

where the summations are over all distinct terms. e.g.

$$\sum x_1x_2 = x_1x_2 + x_1x_3 + \ldots + x_2x_3 + x_2x_4 + \ldots \tag{5.2}$$

Recalling the definition of elementary symmetric funvctions we see that Eq.(5.2) is simply a signed sum over an infinite set of elementary symmetric functions e_n with

$$e_n = m_{1^n} = s_{1^n} = \{1^n\} \tag{5.3}$$

and hence Eq.(5.2) may be written as an infinite sum of $S-$functions such that

$$\begin{aligned} L &= 1 - \{1\} + \{1^2\} - \{1^3\} + \ldots \\ &= \sum_{m=0}^{\infty}(-1)^m\{1^m\} \end{aligned} \tag{5.4}$$

We may define a further infinite series of $S-$functions by taking the inverse of Eq.(5.2) to get

$$\begin{aligned} M &= \prod_{i=1}^{\infty}(1-x_i)^{-1} \\ &= 1 + \{1\} + \{2\} + \ldots \\ &= \sum_{m=0}^{\infty}\{m\} \end{aligned} \tag{5.5}$$

Clearly

$$LM = 1 \tag{5.6}$$

a result that is by no means obvious by simply looking at the product of the two series.

In practice large numbers of infinite series and their associated generating functions may be constructed.

We list a few of them below:

$A = \sum_\alpha (-1)^{w_\alpha}\{\alpha\}$	$B = \sum_\beta \{\beta\}$
$C = \sum_\gamma (-1)^{w_\gamma/2}\{\gamma\}$	$D = \sum_\delta \{\delta\}$
$E = \sum_\epsilon (-1)^{(w_\epsilon+r)/2}\{\epsilon\}$	$F = \sum_\zeta \{\zeta\}$
$G = \sum_\epsilon (-1)^{(w_\epsilon-r)/2}\{\epsilon\}$	$H = \sum_\zeta (-1)^{w_\zeta}\{\zeta\}$
$L = \sum_m (-1)^m\{1^m\}$	$M = \sum_m \{m\}$
$P = \sum_m (-1)^m\{m\}$	$Q = \sum_m \{1^m\}$

(5.7)

where (α) and (γ) are mutually conjugate partitions, which in the Frobenius notation take the form

$$(\alpha) = \begin{pmatrix} a_1 & a_2 & \dots & a_r \\ a_1+1 & a_2+1 & \dots & a_r+1 \end{pmatrix} \tag{5.8a}$$

and

$$(\gamma) = \begin{pmatrix} a_1+1 & a_2+1 & \dots & a_r+1 \\ a_1 & a_2 & \dots & a_r \end{pmatrix} \tag{5.8b}$$

(δ) is a partition into *even parts* only and (β) is conjugate to (δ). (ζ) is any partition and (ϵ) is any self-conjugate partition. r is the Frobenius rank of (α), (γ) and (ϵ).
These series occur in mutually inverse pairs:

$$AB = CD = EF = GH = LM = PQ = \{0\} = 1 \tag{5.9}$$

Furthermore,

$$\begin{aligned} LA = PC = E \quad & MB = QD = F \\ MC = AQ = G \quad & LD = PB = H \end{aligned} \tag{5.10}$$

We also note the series

$$R = \{0\} - 2\sum_{a,b}(-1)^{a+b+1}\begin{pmatrix} a \\ b \end{pmatrix} \qquad S = \{0\} + 2\sum_{a,b}\begin{pmatrix} a \\ b \end{pmatrix} \tag{5.11}$$

where we have again used the Frobenius notation, and

$$\begin{aligned} V = \sum_\omega (-1)^q\{\tilde{\omega}\} \quad & W = \sum_\omega (-1)^q\{\omega\} \\ X = \sum_\omega \{\tilde{\omega}\} \quad & Y = \sum_\omega \{\omega\} \end{aligned} \tag{5.12}$$

where (ω) is a partition of an even number into at most two parts, the second of which is q, and $\tilde{\omega}$ is the conjugate of ω. We have the further relations

$$RS = VW = \{0\} = 1 \tag{5.13}$$

and

$$\begin{aligned} PM = AD = W \quad & LQ = BC = V \\ MQ = FG = S \quad & LP = HE = R \end{aligned} \tag{5.14}$$

■ 5.2 Symbolic manipulation

The above relations lead to a method of describing many of the properties of groups via symbolic manipulation of infinite series of $S-$functions. Thus if $\{\lambda\}$ is an $S-$function then we may symbolically write, for example,

$$\{\lambda/M\} = \sum_m \{\lambda/m\} \tag{5.15}$$

We can construct quite remarkable identities such as:

$$BD = \sum_\zeta \{\zeta\}\cdot\{\zeta\} \tag{5.16}$$

or for an arbitrary $S-$function $\{\epsilon\}$

$$BD \cdot \{\epsilon\} = \sum_{\zeta} \{\zeta\} \cdot \{\zeta/\epsilon\} \tag{5.17}$$

Equally remarkably we can find identities such as

$$\{\sigma \cdot \tau\}/Z = \{\sigma/Z\} \cdot \{\tau/Z\} \quad \text{for} \quad Z = L, M, P, Q, R, S, V, W \tag{5.18a}$$

$$\{\sigma \cdot \tau\}/Z = \sum_{\zeta} \{\sigma/\zeta Z\} \cdot \{\tau/\zeta Z\} \quad \text{for} \quad Z = B, D, F, H \tag{5.18b}$$

$$\{\sigma \cdot \tau\}/Z = \sum_{\zeta} (-1)^{w_\zeta} \{\sigma/\zeta Z\} \cdot \{\tau/\tilde{\zeta} Z\} \quad \text{for} \quad Z = A, C, E, G \tag{5.18c}$$

These various identities can lead to a symbolic method of treating properties of groups particularly amenable to computer implementation.

■ References

For more details see:

1. R C King, Luan Dehuai and B G Wybourne, *Symmetrized powers of rotation group representations* J Phys A: Math. Gen.**14** 2509 (1981)
2. G R E Black, R C King and B G Wybourne, *Kronecker products for compact semisimple Lie groups* J Phys A: Math. Gen. **16** 1555 (1983)
3. R C King, B G Wybourne and M Yang, *Slinkies and the S−function content of certain generating functions* J Phys A: Math. Gen. **22** 4519 (1989)

■ 5.3 The $U_n \to U_{n-1}$ branching rule

As an illustration of the preceding remarks we apply the properties of $S-$functions to the determination of the $U_n \to U_{n-1}$ branching rules. The vector irrep $\{1\}$ of U_n can be taken as decomposing under $U_n \to U_{n-1}$ as

$$\{1\} \to \{1\} + \{0\} \tag{5.19}$$

that is into a vector $\{1\}$ and scalar $\{0\}$ of U_{n-1}. In general, the spaces corresponding to tensors for which a particular number of indices, say m, take on the value n, define invariant subspaces. Such indices must be mutually symmetrised. The irreducible representations specified by the quotient $\{\lambda/m\}$ are those corresponding to tensors obtained by contracting the indices of the tensor corresponding to $\{\lambda\}$ with an $m-$th rank symmetric tensor. Thus we may symbolically write the general branching rule as simply

$$\{\lambda\} \to \{\lambda/M\} \tag{5.20}$$

Thus for example under $U_3 \to U_2$ we have

$$\begin{aligned} \{21\} &\to \{21/M\} \\ &\to \{21/0\} + \{21/1\} + \{21/2\} \\ &\to \{21\} + \{2\} + \{11\} + \{1\} \end{aligned} \tag{5.21}$$

■ 5.4 The Gel'fand states and the betweenness condition

The so-called Gel'fand states play an important role in the Unitary Group Approach (UGA) to many-electron theory. This comes about from considering the canonical chain of groups

$$U_n \supset U_{n-1} \supset \ldots U_2 \supset U_1 \tag{5.22}$$

The states of such a chain follow directly from consideration of Eq.(5.20). Each state may be represented by a triangular array having n rows. There are n entries $m_{i,n}$ with $i = 1, 2, \ldots, n$ corresponding to the usual partition (λ) padded out with zeroes to fill the row if need be. The second row contains $n-1$ entries $m_{i,n-1}$ placed below the first row so that the entry $m_{1,n-1}$ occurs between the entries $m_{1,n}$ and $m_{2,n}$ etc. Each successive row contains one less entry with the bottom row containing just one entry $m_{1,1}$. The number of such states is just the dimension of the irrep $\{\lambda\}$ of U_n.

Consider the irrep of U_3 labelled as $\{21\}$. We find the eight Gel'fand states

$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 1 & \\ & & 2 & & \end{pmatrix} \quad \begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 1 & \\ & & 1 & & \end{pmatrix}$$

$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 0 & \\ & & 2 & & \end{pmatrix} \quad \begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 0 & \\ & & 1 & & \end{pmatrix}$$

$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 2 & & 0 & \\ & & 0 & & \end{pmatrix} \quad \begin{pmatrix} 2 & & 1 & & 0 \\ & 1 & & 1 & \\ & & 1 & & \end{pmatrix}$$

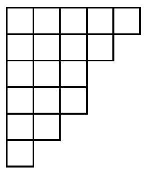
$$\begin{pmatrix} 2 & & 1 & & 0 \\ & 1 & & 0 & \\ & & 1 & & \end{pmatrix} \quad \begin{pmatrix} 2 & & 1 & & 0 \\ & 1 & & 0 & \\ & & 0 & & \end{pmatrix}$$

■ 5.5 The Murnaghan-Nakayama rule for $S(N)$ characters

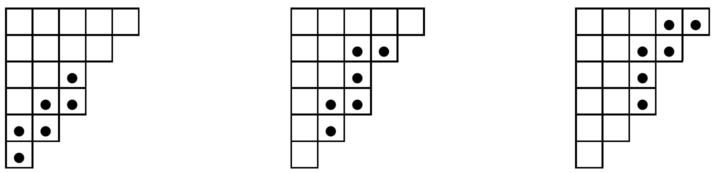
It is not my intention to give anymore than hints at methods of calculating the characters of $S(N)$ a subject well covered in the books of James and Kerber, Littlewood, Murnaghan, Macdonald, Robinson and Sagan but rather to indicate those specialisations that are of immediate application in quantum chemistry. The Murnaghan-Nakayama rule is of particular value in starting practical calculations. The key concept is that of the removal of *rim hook*s or *continuous boundary strip*s from a Young frame. A rim hook is a continuous strip of cells along the boundary of the Young frame which when removed leaves a standard Young frame. The length of the strip is the total number of cells in the rim hook. We associate a *sign* with a given rim hook. If the rim hook involves v cells in the vertical direction then the sign of the rim hook is

$$sgn = (-1)^{v-1} \tag{5.23}$$

As an example consider the Young frame associated with the partition (543321)



Let us now mark the three permissible continuous boundary hooks of length 6 as below



In each case the 6-hook involves four rows and hence the number of vertical cells is $v = 4$ and hence the sign is $sgn = -1$.

■ *The Murnaghan-Nakayama Algorithm* The characteristic $\chi^{\{\lambda\}}_{(\rho)}$ for $S(N)$, where $\{\lambda\}$ is the irrep and (ρ) the class may be determined by

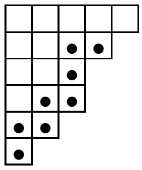
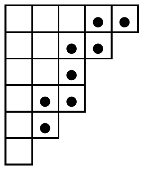
1. Draw the Young frame for the partition λ.
2. Set $i = 1$. Set $sgn\ = +1$.
3. While $\rho_i <> 0$ do begin
4. Remove a rim hook of length ρ_i in all possible ways that leave a standard Young frame. If this is not possible for any of the Young frames then $\chi^{\{\lambda\}}_{(\rho)} = 0$ and the algorithm is terminated.
5. A sign $sgn = sgn * newsign$ is to be associated with each new Young frame created in 3. with $newsign$ being the sign of the rim hook being removed.

6. Set $i = i + 1$
7. End
8. The characteristic $\chi^{\{\lambda\}}_{(\rho)}$ is equal to the sum of the signed units at the termination of the loop.

NB. The result is independent of the order of the removal of the rim hooks.

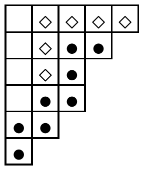
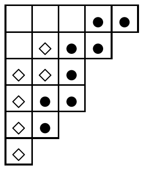
Example of $\chi^{\{543321\}}_{(864)}$

First remove a rim hook of length 8 from the Young frame as shown below

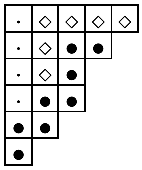
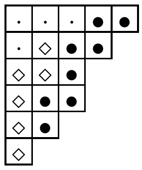
 

In each case the sign of the 8−hook is positive.

Now remove the 6−hook from each of the above two frames to give

Again each 6−hook has a positive sign. Now remove a 4−hook from each frame to give

The sign of each 6−hook is negative and hence each of the frames yields an overall negative sign and hence

$$\chi^{\{543321\}}_{(864)} = -2$$

■ 5.6 The characteristics $\chi^{\{\lambda\}}_{(N)}$

The characteristics $\chi^{\{\lambda\}}_{(N)}$ constitute an important special case. By the Murnaghan-Nakayama rule there is just a single rim-hook of length N to be removed. The only possibility for a non-zero characteristic is if the frame of the partition λ is a single hook of the form $(a1^b)$ with $N = a + b$. The characteristic is thus either null or ± 1. Precisely

$$\chi^{\{\lambda\}}_{(N)} = \begin{cases} (-1)^b & \text{if } \lambda = (a+1, 1^b) \\ 0 & \text{otherwise} \end{cases} \tag{5.24}$$

■ 5.7 The power sum symmetric functions and $S(N)$ characters

The character table of $S(N)$ is the transition matrix $M(p, s)$ that expresses power sum symmetric functions p_ρ as a linear combination of S−functions s_λ with $|\rho| = |\lambda| = N$. Thus

$$p_\rho = \sum_\lambda \chi^\lambda_\rho s_\lambda \tag{5.25}$$

We have the important special case

$$p_n = \sum_{\substack{a,b=0 \\ a+b+1=n}}^{n-1} (-1)^b s_{a+1,1^b} \tag{5.26}$$

Recalling that the power sum symmetric functions are multiplicative we can use Eq. (5.26) to compute all the characteristics associated with a given class by simple application of the Littlewood-Richardson rule. As an example consider the characteristics for the class (31) of $S(4)$. From Eq. (5.26) we have

$$\begin{aligned} p_3 &= \{3\} - \{21\} + \{1^3\} \\ p_1 &= \{1\} \end{aligned}$$

and hence

$$\begin{aligned} p_{31} &= (\{3\} - \{21\} + \{1^3\}) \cdot (\{1\}) \\ &= \{4\} - \{2^2\} + \{1^4\} \end{aligned}$$

showing immediately that the only non-zero characteristics associated with the class (31) are

$$\chi^4_{31} = +1, \qquad \chi^{2^2}_{31} = -1, \qquad \chi^{1^4}_{31} = +1$$

Exercises

1. Generalize the power sum symmetric function to

$$p_n(q;t) = \sum_{\substack{a,b=0 \\ a+b+1=n}}^{n-1} (-1)^q q^a s_{a+1,1^b}(x) \tag{27}$$

and show that

$$p_{31}(q;x) = q^2\{4\} + (q^2-1)\{31\} - q\{2^2\} - (q-1)\{21^2\} + \{1^4\}$$

and for $q = 1$ the $S(4)$ result is recovered. This takes one into Hecke algebras. ([KW1]King and Wybourne, *J. Phys. A: Math. Gen.* **23**, L1193(1990); [KW2]*J. Math, Phys.* **33**, 4 (1992).).

2. Construct a $q-$dependent character table for $N = 3$ and compare it with the corresponding table for $S(3)$. See [KW1].

"It did, Mr Widdershins, until quantum mechanics came along. Now everything's atoms. Reality is a fuzzy business, Mr Widdershins. I see with my eyes, which are a collection of whirling atoms, through the light, which is a collection of whirling atoms. What do I see? I see you Mr Widdershins, who are also a collection of whirling atoms. And in all this intermingling of atoms who is to know where anything starts and anything stops. It's an atomic soup we're in, Mr Widdershins. And all these quantum limbo states only collapse into one concrete reality when there is a human observer"

Pauline Melville, *The Girl with the Celestial Limb* (1991)