Some SCHUR^{TM} Examples I : S–Functions

I. S-Functions: Part 2

Introduction

In this section we illustrate some further features of the SFN mode of **SCHUR**^{TM}. **SCHUR**^{TM} has proved particularly useful in revealing hitherto unnoticed features of symmetric functions. Here we reveal some features of **SCHUR**^{TM} that have exposed aspects of the characteristics of the symmetric group $\mathcal{S}_N$ of significance in quantum chemistry and the so-called Symmetric Group Approach (SGA). The Pauli Exclusion Principle limits interest in $\mathcal{S}_N$ irreducible representations to those describable by just two-row Young diagrams $\{p, q\}$ where

$$p = \frac{N}{2} + S \qquad \text{and} \qquad q = \frac{N}{2} - S \tag{1}$$

with

$$N = p + q \qquad \text{and} \qquad S = \frac{p - q}{2} \tag{2}$$

Thus the characteristics $\chi^{\{p,q\}}_{(\rho)}$ where (λ) is a class of $\mathcal{S}_N$, are of considerable interest. In the following notes we show how **SCHUR**^{TM} can be applied to the calculation of such characteristics and how it can lead to certain conjectures which have subsequently been proved.

Calculation of Characteristics of $\mathcal{S}_N$ using SCHUR^{TM}

The **SCHUR**^{TM} command $< SNchar, n, Class >$ is used to calculate a list of all the non-zero characteristics $\chi^{\{\lambda\}}_{(\rho)}$ where n is the maximum number of parts of the partitions (λ) we wish to consider and (ρ) is the partition designation of the Class of interest. Thus, for example,

```
SFN>

sn2,1^6

      {6} + 5{51} + 9{42} + 5{3^2 }

SFN>
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The integer preceding each S−function $\{p,q\}$ is the characteristic $\chi^{\{p,q\}}_{(1^6)}$ and in this particular case is the dimension of the corresponding irrep of the symmetric group S_6. From Eq. (2) we note that $\{51\}$ is associated with spin $S=2$ and $\{3^2\}$ with spin $S=0$. But these two irreps of S_6 have the same characteristic. This raises the question of when is

$$\chi^{\{p,q\}}_{(1^N)} = \chi^{\{p',q'\}}_{(1^N)} \tag{3}$$

If we use **SCHUR**^{TM} to examine the cases for $N=2,\ldots,14$ we find the equalities given in the table below:-

N	[p,q]S	[p',q']S'	$\chi^{[p,q]}_{(1^N)}$
2	[2]1	[11]0	1
6	[51]2	[33]0	5
7	[52]$\frac{3}{2}$	[43]$\frac{1}{2}$	14
13	[94]$\frac{5}{2}$	[76]$\frac{1}{2}$	429
14	[95]2	[86]1	1001

Inspection of the above table suggests that such equalities are quite rare and appear to divide into two cases

$$N(n) = \begin{cases} n^2+2n-1 & n=1,2,\ldots,\infty \qquad (4a) \\ n^2+2n-2 & n=2,3,\ldots,\infty \qquad (4b) \end{cases}$$

This suggests that the next values of N should occur at $n=4$ giving $N=22$ for case (4b) and $N=23$ for case (4a). Running the **SCHUR**^{TM} commands $<$ sn2, 1^!22 $>$ and

< sn2, 1^!23 > leads to

N	[p,q]S	[p',q']S'	$\chi^{[p,q]}_{(1^N)}$
22	[14 8]3	[12 10]1	149,226
23	[14 9]$\frac{5}{2}$	[13 10]$\frac{3}{2}$	326,876

Now we see a pattern emerging. In case (4a) it appears that

$$p(n) = \frac{n(n+2)}{2}, \quad q(n) = \frac{n(n+1)-2}{2}, \quad p(n)-q(n) = n+1, \quad S = \frac{n+1}{2} \tag{5a}$$

$$p'(n) = \frac{n(n+3)-2}{2}, \quad q'(n) = \frac{n(n+1)}{2}, \quad p'(n)-q'(n) = n-1, \quad S' = \frac{n-1}{2} \tag{5b}$$

while in case (4b)

$$p(n) = \frac{n(n+3)}{2}, \quad q(n) = \frac{n(n+1)-4}{2}, \quad p(n)-q(n) = n+2, \quad S = \frac{n+2}{2} \tag{6a}$$

$$p'(n) = \frac{n(n+3)-4}{2}, \quad q'(n) = \frac{n(n+1)}{2}, \quad p'(n)-q'(n) = n-2, \quad S' = \frac{n-2}{2} \tag{6b}$$

It is left as an exercise to show that the irreps $[p, q]$ and $[p', q']$ as defined in (5a,b) are of the same dimension and likewise for (6a,b). The above gives a complete description of two infinite classes of irreps of S_N

Thus for $N = 118$ we expect from (5a,b) that the two irreps [65 53] and [63 55] will be of the same dimension. This we can readily check in the REP mode of **SCHUR**^{TM} by first setting the group as $S(118)$ and then using **SCHUR**^{TM}'s **dimension** command as shown in the **SCHUR**^{TM} fragment below:-

```
REP mode

REP>

gr s118

Group is S(118)

REP>

dim!65!53

dimension=2617041085391803324124303483690133
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REP>

dim!63,!55

dimension=2617041085391803324124303483690133

REP>
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and likewise for $N = 119$ we expect from (6a,b) that the two irreps [65 54] and [64 55] will be of the same dimension as verified by the **SCHUR**^{TM} fragment below:-

```
REP>

gr s119

Group is S(119)

REP>

dim!65!54

dimension=5323553660882471719158839565113262

REP>

dim!64!55

dimension=5323553660882471719158839565113262

REP>
```

Finally we collect together the results as a single table

N	[p,q]S	[p',q']S'	$\chi^{[p,q]}_{(1^N)}$
2	[2]1	[11]0	1
6	[51]2	[33]0	5
7	$[52]\frac{3}{2}$	$[43]\frac{1}{2}$	14
13	$[94]\frac{5}{2}$	$[76]\frac{1}{2}$	429
14	[95]2	[86]1	1001
22	[14 8]3	[12 10]1	149,226
23	$[14\ 9]\frac{5}{2}$	$[13\ 10]\frac{3}{2}$	326,876
33	$[20\ 13]\frac{7}{2}$	$[18\ 15]\frac{3}{2}$	218,349,120
34	[20 14]3	[19 15]2	463,991,880
46	[27 19]4	[25 21]2	1,335,293,573,130
47	$[27\ 20]\frac{7}{2}$	$[26\ 21]\frac{5}{2}$	2,789,279,908,316
61	$[35\ 26]\frac{9}{2}$	$[33\ 28]\frac{5}{2}$	33,833,779,021,731,045
62	[35 27]4	[34 28]3	69,923,143,311,577,493
78	[44 34]5	[42 36]3	3,527,173,835,643,930,141,670
79	$[44\ 35]\frac{9}{2}$	$[43\ 36]\frac{7}{2}$	7,237,577,480,931,700,810,180
97	$[54\ 43]\frac{11}{2}$	$[52\ 45]\frac{7}{2}$	1,504,860,519,529,865,622,776,830,848
98	[54 44]5	[53 45]4	3,072,423,560,706,808,979,836,029,648
118	[65 53]6	[63 53]5	2,617,041,085,391,803,324,124,303,483,690,133
119	$[65\ 54]\frac{11}{2}$	$[64\ 55]\frac{9}{2}$	5,323,553,660,882,471,719,158,839,565,113,262

Note that the problem is combinatorially explosive. In the preceding we have shown how **SCHUR**^{TM} can lead to conjectures and surprises even in well trodden areas. Of course a conjecture is only a beginning, but it can stimulate efforts towards proof.

An Open Problem

Above we have established two infinite classes of pairs two-row irreps of S_N that have the same dimension. Using **SCHUR**^{TM} shows that there are no other pairs of such two-row irreps of the same dimension. It is an open problem to show whether we have exhausted the possibilities or whether for some higher values of N additional pairs arise, perhaps in a random fashion.

Back to the Future

The next notes will show how **SCHUR**^{TM} has led to new insights into the stabilisation of characteristics of S_N and some hitherto unnoticed identities for two-row characteristics of direct relevance to problems in quantum chemistry and statistical models of spectra. For a preview see:-

Brian G. Wybourne, Norbert Flocke and Jacek Karwowski, "Characters of Two-Row Representations of the Symmetric Group" (draft version only. May 1996) Available at this site.