On general forms for structure of some $[n-1, 1] \otimes [\lambda]$ $\mathcal{S}_n$ inner tensor products with $6 \leq n \leq 20$, (60) for n even, in the context of spin cluster problems of multiquantum NMR

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Consideration of $\mathcal{S}_n$ groups for n even and between $6 \leq n \leq 20$, (60) is consistent with the existence (over a simply reducible (SR) space) of certain similarities in the inner tensor product (ITP) structures associated with $p \leq 2$ $[n-1, 1] \otimes [\lambda]$, or $-\otimes [(n/2)^2]$ products, and for general (even) n for $[n-1, 1] \otimes [n-2, 1^2]$ ITPs, but not for ITPs involving higher general m ($p \leq 3$) components, as in $[n-1, 1] \otimes [n-m, m-1, 1]$. These observations provide considerable insight into the nature of van der Waals ($3 \leq n \leq 20$), metallic-, or "met-carb-" clusters and $n = 12$, 20 cage molecules analogous to dodecahedrane (a cage, $n = 20$ molecule) or ^{13}C buckminsterfullerene(ane) ($n = 60$) $[A]_n$, $[AX]_n$ clusters, besides allowing for further combinatorial views on higher $\mathcal{S}_n$ group characters and their associated group algebra. Mathematical insight to date into the nature of general ITPs involving *non*-SR direct sums has proved less fruitful on account of the number of component partitions spanned by specific ITP maps and their associated multiplicities.

1. Introduction

The study of both stable clusters [1–5] and isodynamic molecules [6,7] or similar van der Waals hydrogen-bonded clusters [8], in terms of their spin statistics [9], rovibrational [10] or wreath product aspects [11,12] has led to a renewed interest in the higher-n symmetric ($\mathcal{S}_n$) groups, as properties central to an understanding of many aspects of cluster physics arising from combinatorial models. In addition to its pertinence to the highly topical areas of *cageo*-^{13}C dodecahedrane [5] and $^{13}C_{60}$ ($[HC]_{60}$) fullerenes(-anes), the related superconducting solid phases of $M_x\,{}^{13}C_{60}$ [1,2], or to $(H_2O)_{20}$ van der Waals clusters [8], there are rather fundamental reasons for interest in higher $\mathcal{S}_n$ groups [12–15] and their inner tensor products (ITPs) [12,15] in the study of multiquantum NMR (MQ-NMR) cluster problems [15], as an aspect of spin dynamics [16].

Both in deriving the nature of carrier spaces associated with the mapping properties under $SU2 \times \mathcal{S}_n$ in the MQ-NMR of stable (multi) cluster problems [15], and in considering the NMR of $(XH_m)_n$ isodynamical clusters [7], higher $\mathcal{S}_n$ symmetric groups play an important role, which we now consider principally for even n within $6 \leq n \leq 20$ (or 60). In addition, knowledge of substructures of the symmetric group allows coherent superpositional bases over Liouville space to be derived; these provide a characterisation of the nature of the pathways for spin coherence transfer [17,18] in MQ-NMR.

Whilst use of cycle-index formulations [7] over $\mathcal{S}_n \downarrow \mathcal{G}$ subduced symmetries [9] may suffice in treating nuclear spin statistics and rovibrational properties of stable clusters, MQ-NMR spin dynamics require one to utilise further aspects [15,19–24] of $\mathcal{S}_n$ symmetry and its ITPs [12]. The latter arise naturally in the formation of Liouville space associated with the spin dynamics of clusters [22,24]. However, the occurrence of explicit υ recoupling terms in Liouvillian $SU2 \times \mathcal{S}_n$ mapping over $\tilde{\mathbb{H}}_\upsilon$ carrier subspaces [20,22] has an additional combinatorial significance; this arises from the observation [15,20,21] that the combinatorial p-tuples associated with $\upsilon \equiv \{\ldots\}(k_1, \ldots, k_n)$ terms under $SU2 \times \mathcal{S}_n$ provide identical information to that which is implicit in the inner direct product formulation of Liouville spaces [15,22,24], i.e. as derived by Latin square construction [19,24] of $\{|kq\upsilon[\tilde{\lambda}]\rangle\rangle\}^q$ from $\{|IM(\,.\,)\rangle\}$ sets of Hilbert space.

Simple $p \leq 3, 4, \ldots$-tuples ($\mathcal{S}_n$) [25] have been found to provide convenient inventory labelling for M subset hierarchies [23] of $\{|IM(\,.\,)\rangle\}$ for $[A]^{(I_i \geq 1)}$ clusters. These give rise to higher dualities, whose unitary group aspects (e.g. for $I \leq 3/2$ and $n \leq 4$) were extensively studied in the early 1980's [26].

2. $-\otimes [n-1, 1]$ SR $\mathcal{S}_n$ – ITP ALGEBRAS from the viewpoint of hooklength formalisms

Reference to any of the standard mathematical treatise on the symmetric group [12] only serves to stress how restricted are the known generalities concerning the full range of ITPs. Hence, we shall consider a specific set of ITPs, namely those derived from $\otimes [n-1, 1]$ products generally with $p \leq 2$-tuplar $\mathcal{S}_n$-irreps, since the resultant direct sum components constitute a simply reducible (SR) subset over the complete $\{[\lambda]\}$ algebra.

Combinatorial arguments play essential roles in defining the feasible operations of isodynamic, or $\mathcal{S}_n[\mathcal{G}]$ wreath product, symmetries of non-rigid van der Waals clusters, besides governing expressions for the components of the generalised characters of representations of $\mathcal{S}_n$ groups. The latter may be obtained directly in terms of combinatorial hooklengths (HL) [27] for modest-n $\mathcal{S}_n$ groups [28,29]. Databases of explicit $20 \geq n \geq 14$ symmetric group properties have been referred to in a recent work of Liu and Balasubramanian [13], using classical Schur symmetric functions [29] [1)] as generators [30]; however, for higher-n symmetric groups, the combinatorical HL formulations [28] certainly are more immediately tractable than the classical approach.

[1)] For other formal symmetric functions, see ref. [30].

Table 1

Structure $[n-1, 1] \otimes [\lambda]$ $(p \leq 2)$ direct products for $\mathcal{S}_n$, $6 \leq n \leq 20$, 60 (all even).

$[n-1,1] \otimes [\lambda]$: $\otimes[\lambda]$	$[n]$	$[n-1,1]$	$[n-2,2]$	$[n-2,11]$	$[n-3,3]$	$[n-3,2,1]$	$[n-3,111]$	$[n-4,4]$	$[n-4,3,1]$	$[n-4,2,2]$	**	$[n-5,5]$	$[n-5,4,1]$	$[n-6,6]$	$[n-6,5,1]$	$[n-7,7]$	$[n-7,6,1]$	$[n-8,8]$	$[n-8,7,1]$	$[n-9,9]$	$[n-9,8,1]$
$[n]$	–	1																			
$[n-1,1]$	1	1	1	1																	
$[n-2,2]$	–	1	1	1	1	1															
$[n-2,1^2]$		1	1	1	–	1	1														a
$[n-3,3]$	–	–	1	–	1	1	–	1	1												
...																					
$[n-4,4]$					1	–	–	1	1	–	*	1	1								
$[n-5,5]$								1	–	–	*	1	1	1	1						
$[n-6,6]$												1	–	1	1	1	1				
$[n-7,7]$														1	–	1	1	1	1		
$[n-8,8]$																1	–	1	1	1	1
$[n-9,9]$																		1	–	1	1..

———; for $\otimes[n-m, m]$ with $m \leq n/2$, whereas ———

for $[n-1, 1] \otimes [(n/2)^2] = [(n/2)+1, (n/2)-1] + [(n/2), (n/2)-1, 1]$; n even

[a]A specific $p \leq 3$ $\otimes[\lambda]$ which exhibits an SR ITP structure over $\{[\lambda]\}$.

On the basis of the specific $\otimes[n-1, 1]$ ITPs summarised in general form in table 1 and the specific $\chi^{[\lambda]}_{(1^n)}(\mathcal{S}_n)$ representational characters of table 2, one may establish the nature and consistency of three general properties for n-even $\mathcal{S}_n$ symmetry. On taking a general condition of $(n/2) > m > 0$, the $[n-1, 1] \otimes [n-m, m]$ ITP becomes an SR direct sum within

$$[n-1,\ 1] \otimes [n-m,\ m] = [n-m+1,\ m-1] + [n-m,\ \ m] + [n-m,\ (m-1),\ 1] + [n-(m+1),\ (m+1)] + [n-(m+1),\ m,\ 1], \qquad (1)$$

whose ITP dimensional order is simply

$$(n-1)(n-2m+1)\, n!/\{m!\,(n-m+1)!\}, \qquad (2)$$

which for $/[n-1, 1] \otimes [\lambda]/$ within $2 \leq m \leq 4$ and arbitrary n takes the respective values

Table 2

Outline of $\chi^{[\lambda]}_{(1^n)}(\mathcal{S}_n) = d_{[\lambda]}$ principal characters over even-n symmetric groups.

$d_{[\lambda]} = /[\lambda]/ \rightarrow$.

n	$[n]$	$[n-1,1]$	$[n-2,2]$	$[n-2,1^2]$	$[n-3,3]$	$[n-3,2,1]$	$[n-3,1^3]$	$[n-4,4]$	$[n-4,3,1]$	$[n-4,2^2]$	*	$[n-5,5]$	$[n-5,4,1]$	$[n-6,6]$	$[n-6,5,1]$	$[n-7,7]$	$[n-7,6,1]$	$[n-8,8]$	$[n-8,7,1]$	$[n-9,9]$
6	1	5	9	10	5	16	10													
8	1	7	20	21	28	64	35	14	70											
12	1	11	54	55	154	320	165	275	891	616	*	297	1408	132	1155					
16	1	15	104	105	440	896	455	1260	3900	2640	*	2548	10752	3640	20020	3432	24960	1430	18018	
18	1	17	135	136	663	1344	680	2244	6885	4641	*	5508	22848	9996	53040	18564	88128	11934	186966	4862
20	1	19	170	171	950	1920	969	3705	11305	7600	*	10659	43776	23256	121125	38760	248064	48450	377910	41990
																			16796	277134
																			$[10^2]$	$[10,9,1]$
60	1	59	1710	1711	32450	64960	32509	453415	1362015	908600	*	4973877								
																((107296E12 −		3814987E9		117788E12
$[-,m]$																(([31, 29],		− $[30^2]$		[30, 29, 1]
$m =$	0	1	2	.	3	.	.	4	.	.		5	.	6	.	7	.	8	.	9

$$\{n(n-1)(n-3)/2\}, \ \{n(n-1)^2(n-5)/6\},$$

and

$$\{(n(n-1)^2(n-2)(n-7)/24\}.$$

For corresponding ITPs involving $[(n/2)^2]$ irreps we have $m = (n/2)$, but now only need to retain the first of the $p \le 2$ and $p \le 3$ (-tuplar) irreps components, since the remaining terms of eq. (1) are outside the 2-tuple bounds. Hence, for even general n,

$$[n-1, 1] \otimes [(n/2)^2] = [(n/2)+1, (n/2)-1] + [(n/2, ((n/2)-1), 1], \tag{3}$$

giving a dimensional order expression of the form

$$(n-1)\, n! / \{(n/2+1)!\,(n/2)!\}. \tag{4}$$

A generalized reduction of the individual orders of the RHS terms of eq. (3) to this form, discussed later, provides additional support for the form of eq. (3).

On examining the analogous $[n-1, 1] \otimes$ ITPs derived from the initial couple of 3-tuplar $\mathcal{S}_n$-partitions, it is seen that of $\otimes [n-m, (m-1)1]$ products, only $[n-1, 1] \otimes [n-2, 1^2]$ gives rise to an SR direct sum over $\{[\lambda]\}$ space within

$$[n-1, 1] \otimes [n-2, 1^2] = [n-1, 1] + [n-2, 2]$$
$$+ [n-2, 1^2] + [n-3, 2, 1] + [n-3, 1^3], \tag{5}$$

where here we restrict discussion to case $n \ge 6$ and even integer values of n. Hence, the dimensional order expression becomes

$$/[n-1, 1] \otimes [n-2, 1^2]/ = (n-2)(n-1)^2/2. \tag{6}$$

The consistency of these relationships may be demonstrated by inspection of tables 1 and 2 within the $\mathcal{S}_n$ group algebras for $n \le 12$, whereas for $14 \le n \le 20$ additional combinatorial data (or database) provides the requisite support for the assertion presented here; the original mathematical conjectures arose from combinatorial reasoning and a specific interest in the properties of simply reducible algebras.

As a demonstration of the assertion of eq. (1), consider m of $[n-1, 1] \otimes [n-m, m]$ over $\mathcal{S}_8$, $\mathcal{S}_{12}$ and $\mathcal{S}_{20}$ for m of, respectively, 3, 5, or 6; the specific equations are

$$/[7, 1] \otimes [5, 3]/(\mathcal{S}_8) = /[6, 2]/ + /[5, 3]/ + /[5, 2, 1]/ + /[4^2]/ + /[4, 3, 1]/$$

$$\text{or} \quad 196 = 20 + 28 + 64 + 14 + 70, \tag{7}$$

$$/[11, 1] \otimes [7, 5]/(\mathcal{S}_{12}) = /[8, 4]/ + /[7, 5]/ + /[7, 4, 1]/ + /[6^2]/ + /[6, 5, 1]/$$

$$\text{or} \quad 3267 = 275 + 297 + 1408 + 132 + 1155, \tag{8}$$

$$/[19,1] \otimes [14,6]/(\mathcal{S}_{20}) = /[15,5]/ + /[14,6]/ + /[14,5,1]/ + /[13,7]/ + /[13,6,1]/$$

$$\text{or} \quad 441\,921 = 10\,659 + 23\,256 + 12\,125 + 38\,760 + 248\,121, \tag{9}$$

and retains the general form of eq. (1), within the analytic dimensionality of eq. (2).

Likewise in the context of eq. (3), the group algebras provide the set of properties such that for a range of $\mathcal{S}_n$ groups,

$$\{/[n-1,1] \otimes [(n/2)^2]/\} \equiv \{25,\ 98,\ 378,\ 1452\}, \qquad \text{for } 6 \le n \le 12 \text{ (even)}, \tag{10}$$

and

$$\{/ \qquad \otimes \qquad /\} \equiv \{21\,450,\ 82\,654,\ 319\,124\}, \qquad \text{for } 16 \le n \le 20 \text{ (even)} \tag{11}$$

as shown in the detailed terms,

$$\begin{aligned} /[11,1] \otimes [6^2]/(\mathcal{S}_{12}) &= /[75)/ + /[651]/ = 297 + 1155, \\ /[19,1] \otimes [10^2)/(\mathcal{S}_{20}) &= /[11,9]/ + /[10,91]/ = 41\,990 + 277\,134. \end{aligned} \tag{12}$$

In addition, the reduction of the dimensional order derived from general RHS irreps of eq. (3) for arbitrary n from

$$n!3\{(n/2-1)!(n/2+2)!\}^{-1} + n!\{(n/2)!(n/2+2)!\}^{-1}2(n/2+1)\,(n/2-1), \tag{13}$$

becomes

$$\begin{aligned} &\{n!/\{(n/2+1)!\,(n/2)!\}\}\,\{3n + (n+2)\,(n-2)\}/(n+4) \\ &\qquad = \{\quad\}\,\{(n-1)\,(n+4)/(n+4)\}; \end{aligned} \tag{14}$$

this provides the form implicit in the LHS of eq. (4) and hence supports the combinatorial arguments underlying the mathematical conjecture.

For specific n, the initial $p \le 3$ partition $[n-2, 11]$ gives rise to the following set of ITP dimensionalities:

$$/[n-1,1] \otimes [n-2,1^2]/ \equiv \{50,\ 147,\ .\ .\ ,\ 605,\ .\ .\ ,\ 1575,\ 2312,\ 3249\};$$

$$\text{for } 6 \le n \le 20. \tag{15}$$

In the $n = 20$ case, we note that

$$/[19,1] \otimes [18,1^2]/ = 19 \times 171 \equiv 19 + 170 + 171 + 1920 + 969 = 3249; \qquad (16)$$

similarly, from hooklength enumerations of specific $\chi^{[\lambda]}_{(.)}(\mathcal{S}_{60})$s, one obtains

$$/[59,1] \otimes [58,1^2]/ = 100\ 949 = 59 + 1710 + 1711 + 64\ 960 + 32\ 509, \qquad (17)$$

in accordance with the analytic dimensional order, eq. (6). However, the task of finding the group algebra for such high-n symmetric groups, even over limited subdomains of characters for $p \leq 2$, 3-tuplar $[\lambda]$s, is not trivial, although in principle, the $\chi^{[\lambda]}_{(.)}$ characters are inherent in hooklength formalisms discussed by both Coleman [28] and in a recent text by Krishnamurthy [30].

In contrast, the $f(p, n)$ structure of the p-tuples is directly accessible using bijective mappings [25,30,31] with

$$\{f(p, 20) \equiv \{1, 10, 33, 64, 84, 90, 82, 70, 54, 42, ..\} \quad 1 \leq p \leq 10, \qquad (18)$$

$$\{f(p, 60) \equiv \{1, 30, 1575, 5260, 12736, ..\} \quad p \leq 5, \qquad (19)$$

and P_{20}, P_{60} Gaussian factors of 627 and 966 467, respectively.

The subsets of $[\lambda]$ partitions contained within the $p \leq 3..$:...: number partitions $\{:n-m, m-2, 1:\}$ or $\{:n-m, m-2, 2:\}$ for $n \leq 20$ symmetric groups have been discussed [32,33] only recently; neither are such ideas to be found in the earlier standard reference works [25,31], to our knowledge.

3. SR-ITPs for n-odd $\mathcal{S}_n$ groups

Whilst the forms of eqs. (1), (3) may be similarly applied with correct $\{[\lambda]\}$ sets generated (as ascertained by $\mathcal{S}_{11}$ from an earlier table [13]), the ITPs derived from $[n-1, 1] \otimes [(n+1)/2, (n-1)/2]$ closest to the centraliser partition differ strongly. In fact, the necessary equation for n odd which replaces eq. (2) has four terms and takes the form

$$[n-1,1] \otimes [(n+1)/2, (n-1)/2] \equiv [n-m+1,\ n-m] + [n-m,\ n-m-1]$$
$$+ [n-m,\ n-m-2, 1] + [(n-m-1)^2, 1] \qquad (20)$$

within

$$/ \otimes / \equiv 2(n-1)\, n! / \{((n-1)/2)!\, ((n+3)/2)!\}. \qquad (21)$$

The continuance of this form to higher odd-n symmetric groups was not examined but may be derived by computation to $n = 17(20)$ from the Balasubramanian database referred to in ref. [13].

4. $-\otimes[(n/2)^2]$ aspects of more general non-SR ITP algebras

For $\otimes[(n/2)^2]$ restricted aspects of ITP algebras for even values $\mathcal{S}_n$ groups, several generalised forms, of SR maps within generally non-SR algebra, may be discerned, including for $\xi = (n/2)$,

$$[n-2, 2] \otimes [(n/2)^2] \to [\xi+2, \xi-2] + [\xi+1, \xi-2, 1] + [\xi^2] + [\xi, \xi-1, 1) + [\xi, \xi-2, 2] + [(\xi-1)^2, 1^2] \tag{22}$$

of dimensional order for even general n,

$$/[n-2, 2] \otimes [(n/2)^2]/ = (n(n-3)/2) \times n!/\{(n/2+1)!(n/2)!\}. \tag{23}$$

By contrast,

$$[n-2, 1^2] \otimes [(n/2)^2] \to [\xi+1, \xi-1] + [\xi+1, \xi-2, 1] + [\xi, \xi-1, 1] + [\xi, \xi-2, 1^2) + [(\xi-1)^2, 2] \tag{24}$$

within the analytical expression for dimensional order,

$$/[n-2, 1^2] \otimes [(n/2)^2]/ = (n-2)(n-1)/2 \times n!/\{(n/2+1)!(n/2)!\}. \tag{25}$$

The detailed combinatorial reasoning behind eq. (22) is contained within the specific even-n symmetric group algebras, as in

$$/[4, 2] \otimes [3^2]/(\mathcal{S}_6) = /[5, 3]/ + /[4, 1^2]/ + /[3^2]/ + /[321]/ . . + /[2^2 1^2]/$$

within

$$45 = 5 + 10 + 5 + 16 + 9, \tag{26}$$

$$/[6, 2] \otimes [4^2]/(\mathcal{S}_8) = /[6, 2]/ + /[5, 2, 1]/ + /[4^2]/ + /[4, 3, 1]/ + /[4, 2^2]/ + /[3^2 1^2]/$$

within

$$280 = 20 + 64 + 14 + 70 + 56 + 56, \tag{27}$$

together with the $\mathcal{S}_{12}$ and $\mathcal{S}_{20}$ relationships,

$$/[10, 2] \otimes [6^2]/ = /[84]/ + /[7, 4, 1]/ + /[6^2]/ + /[6, 5, 1]/ + /[6, 4, 2]/ + /[5^2, 1^2]/$$

within

$$7128 = 275 + 1408 + 132 + 1155 + 2673 + 1485, \tag{28}$$

and

$$/[18,2] \otimes [10^2]/ = /[12,8]/ + /[11,8,1]/ + /[10^2]/ + /[10,9,1]/ + /[10,8,2]/ + /[9^2 1^2]/$$

within

$$2855\,320 = 48\,450 + 413\,440 + 16\,796 + 277\,134 + 1469\,650 + 629\,850. \quad (29)$$

Similarly from the relationships (24), (25), one finds under $\mathcal{S}_6$ and $\mathcal{S}_8$ symmetries

$$/[41^2] \otimes [3^2]/ = /[42]/ + /[41^2]/ + /[3,2,1]/ + /[3,1^3]/ + /[2^3]/$$

for which

$$50 = 9 + 10 + 16 + 10 + 5 \quad (30)$$

and

$$/[61^2]/ \otimes [4^2]/ = /[53]/ + /[5,2,1]/ + /[4,3,1]/ \; /[4,2,1^2]/ + /[3,2^2]/$$

within

$$294 = 28 + 64 + 70 + 90 + 42. \quad (31)$$

The corresponding ITPs under $n = 12$ and 20 symmetric groups, respectively, show

$$/[10,1^2] \otimes [6^2]/ = /[75]/ + /[7,41]/ + /[6,51]/ + /[6,41^2]/ + /[5^2,2]/$$

for

$$7260 = 297 + 1408 + 1155 + 3080 + 1320, \quad (32)$$

and

$$/[18,1^2] \otimes [10^2]/ = /[11,9]/ + /[11,81]/ + /[10,91]/ + /[10,81^2]/ + /[9^2 2]/$$

for

$$2\,872\,116 = 41\,990 + 413\,440 + 277\,134 + 1534\,896 + 604\,656. \quad (33)$$

For odd-values n symmetric group ITP algebra, rather similar combinatorial arguments based on high-n symmetric group trial solutions may well exist to provide us with the analogous relationships to those of eqs. (22)–(25) above, but will require more detailed consideration of the product algebras of $\mathcal{S}_{11}$, $\mathcal{S}_{13}$ and $\mathcal{S}_{15}$ inherent in rather extended group algebras [13], as a consequence of the larger number of partitional components spanned by n-odd $\mathcal{S}_n$ ITP algebras.

5. Mapping relationships between $\mathcal{S}_n$-number partitions and $\mathcal{S}_n$-spin algebras

Applications of the above material arises in two quite distinct mathematical ways for extended spin systems, outlined earlier. The first is concerned with direct generation of Liouville space from $\Gamma(\mathcal{S}_n)$ associated with the analogous spin problem in Hilbert space [34]; in contrast, the second application considers the symmetry inherent in the combinatorial number partitions, $:n - r - r', r, r' \ldots:$ or p-tuple words over either Hilbert spin space, or the explicit Liouville subspaces which derive from recoupling v terms defining the carrier subspace $\{\tilde{\mathbb{H}}_v\}$ set. Both these aspects have been outlined at some length elsewhere [15c, 20, 21]. The latter applications arise from the implicit mapping between a $\mathcal{S}_n$ p-tuple and a specific set of $\mathcal{S}_n$ partitional irreps so that

$$\{ :n-r-r', r, r', \ldots : \} (\mathcal{S}_n) \to R\{[\lambda](\mathcal{S}_n)\}, \tag{34}$$

for R a *correlation* matrix and $\{[\lambda]\}$ a *unit* column vector, as in, for example,

$$\begin{pmatrix} :12: \\ :11,1: \\ :10,2: \\ :10,1,1: \\ :9,3: \\ :9,2,1: \end{pmatrix} \to \begin{pmatrix} 1 & & & & & \\ 1 & 1 & & & & \\ 1 & 1 & 1 & & & \\ 1 & 2 & 1 & 1 & & \\ 1 & 1 & 1 & 0 & 1 & \\ 1 & 2 & 2 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} [12] \\ [11,1] \\ [10,2] \\ [10,1,1] \\ [9,3] \\ [9,2,1] \end{pmatrix} (\mathcal{S}_{12}). \tag{35}$$

As a consequence, there exist various homorphic maps of the p-tuple $\mathcal{S}_n$ words on to $\Gamma(\mathcal{S}_n \downarrow \mathcal{G})$ irreps of a subduced symmetry, with $\{\Gamma'(\mathcal{S}_n \downarrow \mathcal{G})\}$ a unit vector, so that

$$\{ :n-r-r', r, r', \ldots : \} (\mathcal{S}_n) \to R'\{\Gamma'(\mathcal{S}_n \downarrow \mathcal{G})\}, \tag{36}$$

where R' is a further correlation matrix, as in

$$\begin{pmatrix} :10,1,1: \\ :9,2,1: \end{pmatrix} \to \begin{pmatrix} 3 & 8 & 11 & 7 & 7 \\ 11 & 44 & 55 & 33 & 33 \end{pmatrix} \Gamma'(\mathcal{S}_{12} \downarrow \mathrm{A}_5) \tag{37}$$

for Γ' a unit vector over the irreps of the subduced symmetry.

The results of such combinatorial mathematical models, with their marked similarity to the classical combinatorial problem [30] of distinct coloured non-identical balls, is the derivation of maps,

$$[\lambda](\mathcal{S}_n) \to \Gamma(\mathcal{S}_n \downarrow \mathcal{G}), \tag{38}$$

a subduced symmetry correlation property frequently appended to $\mathcal{S}_n$ character tables. Hence, eqs. (35), (38) yield the detailed correlations

$$\begin{pmatrix} [12] \\ [11,1] \\ [10,2] \\ [10,1,1] \\ [9,3] \\ [9,2,1] \end{pmatrix} \to \begin{pmatrix} 1 & & & & \\ . & . & 1 & 1 & 1 \\ 2 & 4 & 6 & 1 & 1 \\ . & 4 & 3 & 4 & 4 \\ 2 & 12 & 10 & 9 & 9 \\ 4 & 20 & 28 & 16 & 16 \end{pmatrix} \begin{pmatrix} \mathcal{A} \\ \mathcal{G} \\ \mathcal{H} \\ \mathcal{T}_1 \\ \mathcal{T}_3 \end{pmatrix} (\mathcal{S}_{12} \downarrow \mathrm{A}_5). \tag{39}$$

Similar maps for $\mathcal{S}_n$, $n = 5, 6, 7, 12$ and 20 have been derived and discussed elsewhere, and summarized in refs. [15,21]. Equation (39) extends the earlier conclusions of Balasubramanian et al. [9b], both in focusing on the insertion of $[\lambda](\mathcal{S}_{12})$ irreps into the symmetry chain between SU2 and $\Gamma(\mathcal{S}_{12} \downarrow A_5)$, and by its ability to derive subduced irreps associated with higher p-tuplar component irreps of the $\mathcal{S}_{12}$ algebra. Naturally, the subduced symmetry associated with specific $\mathcal{S}_{12}$ number partitions (p-tuples) provides firm evidence for the latter's $[\lambda]$ partitional decomposition within the mappings discussed above in eq. (35).

6. Nature of applications of $\mathcal{S}_n$ ITP algebras and concluding remarks

Interesting recent experimental work on "met-carb" pentagonal dodecahedral clusters $[Ti_8C_{12}]$ [35] (but as a ^{13}C cluster), as well as solid-state work on ^{13}C-cubane (mainly in a plastic phase) [36], offer examples of unusual spin clusters, $[A]_8^{5/2} \otimes [X]_{12}$ spin system under $\mathcal{S}_{12} \downarrow T$ and $[AX]_8$ (liquid state) problem under $\mathcal{S}_8 \downarrow O$ finite group symmetries, respectively. In addition, the borohydride ion $[^{11}BH]_{12}^{2-}$ species has been reconsidered [15,32]; the multinuclear $M_x(^{13}Co)_nL$ diamagnetic coordination clusters for $n = 15, 18$ and $M = $ Pt, Rh, Ru of ref. [4c] provide further unusual subduced spin symmetry problems of possible NMR interest. These comments serve to stress the existence of extended spin cluster problems providing additions to earlier work [26,34].

Further consideration of other aspects of non-SR ITP algebras is deferred, since it is more pertinent to related work on met-carba and cage ions [37].

Both as an auxiliary group of SU unitary symmetry and especially within $SU \times \mathcal{S}_n$ duality, it is well known from the work of Li and Paldus [38] and from the properties of boson pattern algebra [39], that the $\mathcal{S}_n$ group provides a particularly direct insight into angular momentum physics of many-spin problems with their associated scalar invariants. Such ideas carry over into our understanding of multi-quantum coherence transfer in MQ-NMR on noting the existence of a Heisenburg superalgebra over s_i bosons [19,20] derived from commutator properties of super-operators inherent in spin dynamical formalisms.

Indeed, such ideas allow the formulation [20] of Yamanouchi index tensorial bases and Wigner fundamental unit superoperators over tensorial bases of even 0 and 2 $(=\tilde{1})$ k_i indices over the augmented space for more extended problems than the few body $SU2 \times \mathcal{S}_3$ interactions, whose non-square unit tensor operators [40], generating well-known NMR angular momenta coupling ideas, have been discussed purely from the standpoint of unitary algebra. The language of cooperative duality over simple reducible Liouville carrier subspaces [19] offers greater insight, since it draws on the scalar invariant properties associated with $\mathcal{S}_n$ groups [22–24,41].

Finally, on the purely symmetric group aspects, clearly the analytic and other expressions for the dimensional order of ITP algebras provide strong support for our combinatorial reasoning about regular ITP structure for $\mathcal{S}_n$ groups having n

greater than the number of component irreps spanned by specific ITPs. Mathematical conjectures about the corresponding regularities for non-SR ITP algebras are more difficult and require detailed knowledge of still higher $\mathcal{S}_n$ groups; further physical insight from a combinatorial approach without the need to compute the full product algebra may yet be available from a wider dissemination of Liu and Balasubramanian's descriptions of the characters of the $\mathcal{S}_n$ groups [13] for $n < 18, ..(20)$.

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References

[1] R. Cohen and W.E. Pickett, Phys. Rev. Lett. 64(1990)2575.
[2] S.C. Erwin and E. Pederson, Phys. Rev. Lett. 67(1991)1610;
P.W. Stephens, Nature 351(1991)632.
[3] D.W. Kroto and R.E. Smalley, Nature 318(1985)162.
[4] R. Tycho, R. Haddon, D.C. Douglas and A. Mujsic, J. Phys. Chem. 95(1991)518;
R.E. Smalley, in: *Atomic and Molecular Clusters*, ed. E. Bernstein (Elsevier, Amsterdam, 1990);
D.M. Mingos and D.J. Wales, *Introduction to Cluster Chemistry* (Prentice–Hall, Englewood Cliffs, 1990).
[5] L. Paquette, R.J. Ternansky, D. Balogh and G. Kentgen, J. Am. Chem. Soc. 105(1983)5441.
[6] H.C. Longuet-Higgins, Mol. Phys. 6(1963)445;
K. Balasubramanian, J. Chem. Phys. 72(1980)665; 73(1980)3321; 78(1983)6358.
[7] K. Balasubramanian, J. Chem. Phys. 95(1991)8273.
[8] S. Wei, Z. Shi and A.W. Castleman, J. Chem. Phys. 94(1991)3268.
[9] K. Balasubramanian, Chem. Phys. Lett. 183(1991)292; 200(1992)649; 202(1993)271.
K. Balasubramanian, K.S. Pitzer and H.L. Strauss, J. Mol. Spectry. 93(1982)447.
[10] W.G. Harter and D.E. Weekes, J. Chem. Phys. 90(1989)4726.
[11] K. Balasubramanian, Chem. Rev. 88(1985)599, and references therein.
[12] G.B. James and A. Kerber, *Representations of $\mathcal{S}_n$ Group* (Addison/CUP, Reading, 1982).
[13] X. Liu and K. Balasubramanian, J. Comput. Chem. 10(1989)417.
[14] M. Ziauddin, Proc. Lond. Math. Soc. 42(1936)340.
[15] J.P. Colpa and F.P. Temme, Chem. Phys. 154(1991)97; *Proc. Coll. Ampère XXV* (Springer, Berlin, 1990) p. 691; Phys. Z. B89(1992)335.
[16] B.C. Sanctuary and T.K. Halstead, in: *Advances in Optical and Magnetic Resonance*, Vol. 15 (Academic Press, New York, 1991), and references therein.

[17] F.P. Temme, J. Magn. Reson. 83(1989)383.
[18] F.P. Temme and J.P. Colpa, Mol. Phys. 73(1991)953.
[19] F.P. Temme, Physica A (1993), in press; J. Math. Phys. 32(1991)1638.
[20] F.P. Temme, Z. Phys. B80(1992)83.
[21] F.P. Temme and J.P. Colpa, Z. Phys. D25(1992), in press.
[22] F.P. Temme, Physica A166(1990)676.
[23] F.P. Temme, Physica A166(1990)685; Mol. Phys. 66(1989)1075.
[24] F.P. Temme, Chem. Phys. 132(1989)9.
[25] C. Berge, *Principles of Combinatorics* (Dunod/Academic, Paris/London, 1976);
G.C. Rota, in: *Finite Operator Calculus* (Academic Press, London, 1976);
A.Z. Mekjian and S.J. Lee, Phys. Rev. A44(1991)6294.
[26] R.L. Flurry and T.H. Siddall, Phys. Rev. B31(1985)4153, and references therein.
R.D. Kent, M. Schlessinger and P. Ponnapoulis, Phys. Rev. B31(1985)1264.
[27] J.S. Frame, G. de Q Robinson and R.M. Thrall, Canad. J. Math. 6(1954)316.
[28] A.J. Coleman, *Induced Symmetry Applied to* $\mathcal{S}_n$ *and GL(n) Groups* (Queen's Mathematical Publ., Ontario, 1964); *Advances in Quantum Chemistry*, Vol. 4 (Academic Press, London, 1968) p. 83 ff.
[29] W. Ledermann, *Introduction to Group Characters*, 2nd Ed. (Cambridge University Press, Cambridge, 1987).
[30] V. Krishnamurthy, *Combinatorics and its Applications* (Ellis Horwood/E–W Press, Chichester/New Delhi, 1988);
M. Randić, J. Math. Chem. 1(1987)145.
[31] G.E. Andrews, *Number Partitions* (Academic Press, New York, 1976).
[32] F.P. Temme, Chem. Phys. Lett. 200(1992)534.
[33] J.P. Colpa and F.P. Temme, J. Math. Chem. 11(1992)341.
[34] P.L. Corio, *The Structure of High Resolution NMR* (Academic Press, New York, 1967); refs. [16] and [24].
[35] B. Guo, K.P. Kerns and A.W. Castleman, Science 255(1992)1411.
[36] M.A. White, R. Wasylishen, P. Eaton, K. Prasad and N. Nodari, J. Phys. Chem. 96(1992)421.
[37] F.P. Temme, Mol. Phys. 78(1993), in press;
F.P. Temme, C.E. Mitchell and M.S. Krishnan, Mol. Phys. (1993), in press.
[38] X. Li and J. Pauldus, Int. J. Quant. Chem. 36(189)127.
[39] J.D. Louck and L.C. Biedenharn, in: *The Permutation Group in Physics and Chemistry*, ed. J. Hinze (Springer, Berlin, 1979) pp. 121 ff, 148 ff; also, works cited in refs. [19], [20].
[40] G.J. Bowden and M.J. Prandolini, Mol. Phys. 74(1991)985, 999.
[41] J.M. Levy-Leblond and N. Levy-Nahas, J. Math. Phys. 6(1965)1372.