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SUMMARY OF $\mathcal{S}_n$ MAPPING PROPERTIES OF SOME LEXICAL p-TUPLES, OR WORDLENGTHS, OVER (M_1–M_n) FIELDS OF ROTA–CAYLEY ALGEBRA IN GENERATING HILBERT SPACE $SO(3)\times\mathcal{S}_n$ IRREPS OF HIGHER I_i IDENTICAL SPIN CLUSTERS, $[A]_n(\mathcal{S}_n)$, FOR $n\leq 7$

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Abstract

Subdomain partitioning of n-fold fields associated with $\mathcal{S}_n$-scalar invariants of Rota–Cayley algebra and enumerative combinatorics are shown to provide direct access to the hierarchical substructure (inventory) of higher identical spin clusters. Such lexical methods based on p-tuples are especially valuable in treating higher I_i spin cluster bases. On examining dimensionality criteria, in the context of inner tensor product (ITP) algebra, they clarify the nature of such spin bases under $SO(3)\times\mathcal{S}_n$ dualities involving extended symmetric groups and their related $\mathcal{S}_n\downarrow\mathcal{G}$ subduced symmetries for $5\leq n\leq 7$ in the context of multiquantum NMR, using simple combinatorial arguments. The present work reports the conceptual aspects of monocluster substructures over Hilbert space underlying our recent papers on bicluster spin dynamics over $\mathcal{S}_n$-partitioned Liouville space. The substructure of $[^2D]_n(\mathcal{S}_n)$ spin systems over $\{[\lambda]\}$ sets derived here may be utilized in direct product subsets $\{[\lambda]\}^q$ pertinent to the partitioned Liouvillians describing the spin dynamics of $[^{11}BD]_6^{2-}$ and $[^{11}BD]_7^{2-}$ cage ions.

1. Introduction

Scalar invariants of Cayley algebra *over an n-fold field* [1] may be written in terms of combinatorial p-tuples , or "generalized (lexical) wordlengths" (GWL), based on the enumerative combinatoricals [2] of our earlier conceptual discussions [3–5]. These provide powerful tools with which to examine the substructure of a variety of spin clusters under the symmetric group $\mathcal{S}_n$. In addition to $\mathcal{S}_2$, $\mathcal{S}_3$, and $\mathcal{S}_4$ spin problems, application of these ideas to the higher-n $\mathcal{S}_n$ groups is of value in the context of clusters and molecular cage ions; however, any discussion of $n\geq 5$ fold spin clusters necessarily requires a consideration of $\mathcal{S}_n\downarrow\mathcal{G}$ subduction to yield the irreducible representations (irreps) of some subgroup of the pertinent symmetric group. In the context of multiquantum NMR (MQ-NMR) of cage-cluster ions constituting bicluster spin systems, the mapping associated with subduction allows us to consider the spin cluster systems $[AX]_n(\mathcal{S}_n)$ for $n = 6, 7$ as models for $[^{11}B\tilde{H}]_n^{2-}$ ions [4,5]. Within dual subduced symmetry irreps over partitioned $\{|kqv[\tilde{\lambda}]\rangle\rangle\}$ operator bases of Liouville space [3] associated with the quantum Liouville equation, factoriza-tion of the Liouvillian of the full spin problem into subproblems of reduced order becomes possible and a motivation for the present line of enquiry.

For $I_i \geq 1$ clusters in the context of conventional Hilbert spin space, the simple directness of the combinatorial method over n-fold lexical fields has special value when compared to earlier Racah methods [6,7] of treating dual irreps under $SO(3) \times \mathcal{S}_n$ duality associated with higher identical spins. This suggests that our intermediate implicit results, as derived in the course of our examination of the Liouville space substructure of two (^{11}B) borohydride MQ-NMR problems [4], deserve to be presented in their own right.

The present note summarizes the application of p-tuples, i.e. lexical words over $\mathcal{S}_n$-fields (referred to as number partitions in the mathematical literature) for $n \leq 7$ monoclusters as a form of hierarchical model, whose individual components introduce convenient lexical labelling comparable to the physical models under the class algebra of the subgroup associated with subduction. Hence, the associated $\mathcal{S}_n \rightarrow \mathcal{S}_n \downarrow \mathcal{G}$ mappings specify the irrep substructure over Hilbert space derived from $[A]_n^{(I_i = 1)}$ clusters. However, it is the properties of the p-tuple or lexical GWL under the general $\mathcal{S}_n$ symmetric group within Rota's view of Cayley algebra over an n-fold field [1] that constitutes the essence of the method adopted here.

Prior to embarking on the essentials of the presentation, some mention of the wider value of spin symmetry in contexts other than MQ-NMR may be helpful. In particular, knowledge of the irreps associated with the tetrahedral perdeutero-ions X-d_4 [8,9] or of octahedral cations [10,11], such as $(^{14}N\text{-}d_3)_6M^+$, is strongly pertinent to quantum rotational tunnelling [12] exhibited by molecular solids [13], since the physical processes resulting in spin conversion are inherently spin permutation under the symmetry group. Additional aspects of quantum rotational tunnelling in collinear bis-triadic CH_3 or CD_3 systems [14] may be found in the recent work of Clough [15] on topological phases, and of Fillaux and Carlile [16] on the sin-Gordon-like behaviour of one-dimensionally ordered solids. Our understanding of low temperature models of quantum rotational phenomena arises from studies of both NMR and spin-dependent neutron scattering phenomena.

The non-simple reducibility (NSR) of $SO(3) \times \mathcal{S}_n$ spin spaces associated with $I_i \geq 1$ is in contrast to the induced-symmetry properties inherent under the $SU2 \times \mathcal{S}_n$ groups discussed by Coleman [17], but presents no problem in deriving irreducible representations (irreps) under the group for the modest $n \ll 12$ used here. Dimensionality arguments and other criteria are invoked in deriving the expansion over the $\{[\lambda]\}$ set of the $p \leq (2I_i + 1)$-tuple as a mathematical model. In addition, the $\mathcal{S}_n$-inner tensor products (ITP), as a part of the group algebra [18], allow one some insight into which $[\lambda]$ components of the spin space and -tuple are multiple, or zero, elements of the field for $I_i > 1/2$. It is notable that the combinatorial aspects of lexical hierarchies take on greater structure as I_i increases [3] for any n-fold $[A]_n$ spin cluster.

2. Outline of method and notation

To orientate the reader, we start with the rather simple p-tuples of $\mathcal{S}_n$ for $n \leq 4$ before considering $[A]_5(\mathcal{S}_5)$, $[A]_6(\mathcal{S}_6)$, and $[A]_7(\mathcal{S}_7)$ spin-one cluster problems. We stress throughout various mapping aspects for $p \leq 3$ -tuples defining these clusters, where they arise from a hierarchical inspection process under the constraint imposed by z-projection, or M-weight, labelling of the subspace, as outlined in ref. [3]; the notation of the second paper of ref. [3] is retained here. Thus, the p term implies that the number of subfields is p and that each contains a set of local identical labels into which the total $\mathcal{S}_n$-Cayley field is subdivided; the corresponding -tuples, lexical wordlengths, are denoted by $:mr:$ or $:mrr':$ for $p \leq 2, 3$, respectively, where these GWL span ($\overset{\frown}{\forall}$) the n-fold field associated with Cayley algebra and readily map (denoted by conventional $\longrightarrow$) onto the irreps of the pertinent $\mathcal{S}_n$ group. Discussion of the lexical model invariances under cycle or class operators of the subgroup [4] leads one directly to the subduced $\mathcal{S}_n \downarrow \mathcal{G}$ irreps.

Additional notational points concern the use of /../ for group order, or irrep character $\chi^{[\lambda]}_{1^n}$ (degeneracy), and $n^{(M)}$ for the subdimensionalities of a specific M spin cluster subspace, while $\{..\}$ braces describe (corresponding) set(s) of -tuples or irreps, frequently in order from highest M weights. Finally, we stress our use of unit (column) vectors containing the lexical -tuples or $\mathcal{S}_n$-irreps (shown as £), or subgroup irreps (denoted ₣′) in either dictionary $\{[n], [n-1, 1]..\}$ order, or (for Γ) conventional order.

Hence, under $\mathcal{S}_2$–$\mathcal{S}_4$ spin symmetries the $p \leq 3$-tuples, for $I_i = 1$ clusters, map onto the Hilbert space irreps $[\lambda](\mathcal{S}_n)$ in the following manner:

$$:2: \longrightarrow [2]; \ :1^2: \longrightarrow [2] + [1^2], \tag{1a}$$

so that over full $\{|IM\alpha\rangle\}$ space under $\mathcal{S}_2 \times SO(3)$, the total subdimensionalities $n_{\Sigma[\lambda]}$ for $M = 2, 1, 0$, respectively, span

$$\left\{n_{\sum[\lambda]}\right\}^M \quad \overset{\frown}{\forall} \ \{1, 2, 3\}, \tag{1b}$$

yielding over a $(2I_i + 1)^n = 3^n$-fold space of the total spin irrep for $\Gamma^{(I_i = 1)}$,

$$\Gamma = 6[2] + 3[1^2]. \tag{1c}$$

Likewise for $[A]_3(\mathcal{S}_3)^{(I_i = 1)}$, mappings from GWL$(\mathcal{S}_3)$ take the form

$$:3: \longrightarrow [3]; \ :21: \longrightarrow [3] + [21] \tag{2}$$

within the scheme

$$\begin{aligned} &\{:3:; \ :21:; \ 2:21:; \ :1^3: + :3:\} \\ &\quad \overset{\frown}{\forall} \ \{[3]; [3] + [21]; 2[3] + 2[21]; 2[3] + 2[21] + [1^3]\} \end{aligned} \tag{3}$$

over $M = 3$ (down to 0) subspaces having subdimensionalities 1, 3, 6, and 7, within a 27-fold dimensional total spin-one space under $SO(3) \times S_3$.

The $[A]_4^{(I_i=1)}(S_4)$ cluster spans a $3^4 = 81$-fold total spin space with {1, 4, 10, 16, and 19} subdimensionalities in the positive M domain as determined by the 3-tuple (S_4) properties,

$$:2^2: \rightarrow [4] + [2^2] + [31],$$

$$:21^2: \rightarrow [4] + [2^2] + [21^2] + 2[31] \tag{4}$$

within the lexical word structure of M space,

$$\{ :4:, :31:, :2^2: + :31:, :21^2: + :31:, :4: + :21^2: + :2^2: \}. \tag{5}$$

Hence, one obtains the irreps over $4 \geq M \geq 0$ subspaces as a column vector,

$$\{\Gamma(S_4)\}^M = \begin{pmatrix} [4] \\ [4] + [31] \\ 2[4] + [2^2] + 2[31] \\ 2[4] + [2^2] + [21^2] + 3[31] \\ 3[4] + 2[2^2] + [21^2] + 3[31] \end{pmatrix}. \tag{6}$$

Clearly, the remaining GWL(S_4), on the basis of dimensionality arguments, maps onto the following irreps:

$$:1^4: \rightarrow [4] + [1^4] + 2[2^2] + 3[21^2] + [31]. \tag{7}$$

However, this is a $p \leq 4$-tuple, only needed in treating $I_i \geq 3/2$ cluster problems. Additional higher I_i clusters irreps over (M_1–M_4) for high outer M and the corresponding Liouville space irreps over (k_1–k_4) under S_4 for outer q subspaces are summarized elsewhere [3].

Before discussing the higher-n symmetric group aspects, we noted that general χ_E invariances may be associated with the mathematical lexical models for wordlengths $:mr:$, $:mrr':$, . . . , i.e. GWLs of specific p (i.e. for number of subfields of GWL, or -tuple, within $n = m + r$, or $n = m + r + r' + \ldots$) with

$$\left\{ :mr:,\ p \leq 2,\ \chi_E \equiv \binom{n}{r} \right\}, \tag{8a}$$

$$\left\{ :mr'r'':,\ p \leq 3, \equiv \prod \binom{n}{r} \binom{r = r' + r''}{r''} \right\}, \tag{8b}$$

where the notation $\binom{n}{r}$ refers to a combinatorial factor and $/:\ldots:/ \equiv \chi_{\rm E}$. Hence, the additional combinatorial factor of eq. (8b) for $p = 3$ is a simple product of combinatorial binomial factors for binary choices associated with probabilities within the full field and from within a residual subfield. For $p \leq 2$ GWLs of form $:n-r, r:$, the set of corresponding $p \leq 2$ partitions $\{[n]\,..\,[n-r, r]\}$ is both simple-reducible and complete up to the lexical form of the specific -tuple.

The only remaining point of interest in $p \leq 2$ words and $[\lambda]$'s is concerned with the question of mapping onto the subduced symmetry irreps which is best considered in terms of the invariance properties of the set of 2-tuples in decreasing order, $\{:n:, :n-1, 1:, \ldots :(n/2)(n/2):\}$, a hierarchical mathematical model.

The analogy in eqs. (8) to the series that eventually gives rise to monomials, and thus to umbral algebra, is of some mathematical interest*; however, specialist knowledge of combinatorics is not needed to utilise the enumerative techniques outlined here. Dimensionality and consistency relationships building from the lower p forms of p-tuples within the subduced symmetry suffice.

3. Application to extended $\mathcal{S}_n$ groups, $5 \leq n \leq 7$

A study of the inner tensor products (ITP) of the $\mathcal{S}_5$–$\mathcal{S}_8$ groups, utilizing the tabulations in ref. [18], is a valuable preliminary to any consideration of p-tuple decompositions under $\mathcal{S}_n$. On writing $\mathcal{E}(\mathcal{S}_n, p)$ for a *unit* vector over a lexical set of partitions under a prime, e.g. of $p \leq 3$, the full sets become

$$\{[5], [41], [32], [31^2], [2^21]\}(\mathcal{S}_5, p \leq 3),$$

$$\{[6], [51], [42], [41^2], [3^2], [321], [2^3]\}(\mathcal{S}_6, p \leq 3), \tag{9}$$

$$\{[7], [61], [52], [51^2], [43], [421], [3^21], [32^2]\}(\mathcal{S}_7, p \leq 3).$$

On the basis of dimensionality, uniqueness and correspondence to invariance properties over the hierarchy of p-tuple models, the mapping of 3-tuple of order $/:\ldots:/$ onto the full $p \leq 3$ irreps set under the $\mathcal{S}_5$ group becomes

$$:31^2: \rightarrow (1, 2, 1,)\,\mathcal{E}(\mathcal{S}_5, p \leq 3), \qquad /:.:/ = 20, \tag{10}$$

$$:2^21: \rightarrow (1, 2, 2, 1, 1\,)\,\mathcal{E}, \qquad /:.:/ = 30, \tag{11}$$

within the invariance properties discussed earlier [19]. The p-tuple hierarchy, or inventory, which gives rise to the $SO(3) \times \mathcal{S}_5$ bases over outer M of table 1, is given in the appendix.

*See comments of Rota et al. referred to in the concluding paragraph.

Table 1

The SO(3) × $\mathcal{S}_5$ hierarchical substructure over outer M weight (z-projection) for the fivefold spin-one cluster.

M	[5] $/../=1$	[41] $/../=4$	[32] $/../=5$	[31^2] $/../=6$	[2^21] $/../=5$	$n^M_{\Sigma[\lambda]}$
5	1					1
4	1	1				5
3	2	2	1			15
2	2	3	2	1		30
1	3	4	3	1	1	45
0	3	4	3	2	1	51
Σ	21	24	15	6	3	243

Under the $\mathcal{S}_6$ group, the decompositional mapping proceeds as

$$:41^2: \rightarrow (1, 2, 1, 1)\pounds(\mathcal{S}_6, p \leq 3), \qquad /:..:/ = 30, \tag{12}$$

$$:321: \rightarrow (1, 2, 2, 1, 1, 1)\pounds, \qquad /:..:/ = 60, \tag{13}$$

$$:2^3: \rightarrow (1, 2, 3, 1, 1, 2, 1)\pounds, \qquad /:..:/ = 90. \tag{14}$$

Thus, the $[\mathrm{A}]_6^{(I_i=1)}$ cluster is found to span the irreps of the total space,

$$\Gamma = (28, 35, 27, 10, 10, 8, 1)\pounds(\mathcal{S}_6, p \leq 3), \tag{15}$$

where the substructure of irreps over M takes the form depicted in table 2. The actual lexical word structure of $\{|IM\alpha\rangle\}$ space is derived in a manner similar to that summarized [3] for $I_i \leq 5/2$ clusters. The additional mappings which take one from $[\lambda](\mathcal{S}_n)$ to $\Gamma'(\mathcal{S}_n \downarrow \mathcal{G})$ subduced symmetry for $\mathcal{S}_6$, $\mathcal{S}_7$ are discussed in ref. [4]; they are given in an appendix to complete our statement of mapping properties under these spin symmetries.

For the $\mathcal{S}_7$ group, similar inner tensor product consideration lead one to map the GWLs onto the irrep spin space within

$$:51^2: \rightarrow (1, 2, 1, 1)\pounds(\mathcal{S}_7, p \leq 3), \tag{16}$$

$$:421: \rightarrow (1, 2, 2, 1, 1, 1)\pounds, \tag{17}$$

$$:3^21: \rightarrow (1, 2, 2, 1, 2, 1, 1)\pounds, \tag{18}$$

$$:32^2: \rightarrow (1, 2, 3, 1, 2, 2, 1, 1)\pounds, \tag{19}$$

over a set of dimensionalities $\{/:..:/\}$ of 42, 105, 140 and 210, respectively.

Table 2

The partitional substructure over M subspaces associated with duality of the $[A]_6^{(I_i=1)}(SO(3) \times \mathcal{S}_6)$ spin cluster, together with their subdimensionality over M and the principal characters $\chi_{1^n}^{[\lambda]}$ of the individual partitions under the group, denoted $/[..]/$.

M	[6] $/../=1$	[51] $/../=5$	[42] $/../=9$	[41^2] $/../=10$	[3^2] $/../=5$	[321] $/../=16$	[2^3] $/../=5$	$n^M_{\Sigma[\lambda]}$
6	1							1
5	1	1						6
4	2	2	1					21
3	2	3	2	1	1			50
2	3	4	4	1	1	1		90
1	3	5	4	2	2	2		126
0	4	5	5	2	2	2	1	141
Σ	28	35	27	10	10	8	1	729

Hence, the 2187-fold spin space of $[A]_7(\mathcal{S}_7)^{(I_i=1)}$ spans the irrep hierarchy over M shown in table 3 within the appropriate detailed lexical structures of the second paper of ref. [4]; as a consequence of the above mappings, the total irreps for the monocluster $[A]_7(\mathcal{S}_7)$ span

$$\{36, 47, 43, 15, 24, 15, 6, 3\}\,\pounds(\mathcal{S}_7,\, p \leq 3), \tag{20}$$

which in turn map onto the $\mathcal{S}_7 \downarrow D_5$ subduced symmetry (unit) irreps F' to give

$$\Gamma' = (270, 189, 432, 432)\mathrm{F}'. \tag{21}$$

Equations (9)–(20) bring together aspects of p-tuples underlying various recent papers by the present authors [4,19] on bicluster $[AX]_n$ and other spin cluster systems.

Now we are in a position to derive the full spin irreps for the components of the high temperature model of $(^{14}NH_3)_6$–M hexamino–metal cations as

$$((28, 35, 27, 10, 10, 8, 1)\pounds(\mathcal{S}_6,\, p \leq 3)) \otimes \Gamma(\otimes(\Gamma^{(I_i=1/2)}(\mathcal{S}_3))_6), \tag{22}$$

where the first term of the direct product is associated with aspects of the $I_i = 1$, ^{14}N spin cluster. At lower temperatures (20–170 K) there may be a dynamical aspect involved as well as tunnelling processes, requiring the introduction of the general wreath product spin symmetry [20], as typified by the $\{(NH)_3\}_n$ clusters considered recently by Balasubramanian [21].

Caution is necessary in applying symmetrization techniques to bases pertaining to certain types of NMR experiments such as commonly utilised in studying tunnelling

Table 3

The corresponding dual partitional hierarchy and its subdimensionalities over M subspaces of the $[A]_7$ identical spin-one cluster.

M	[7] $/../=1$	[61] $/../=6$	[52] $/../=14$	$[51^2]$ $/../=15$	[43] $/../=14$	[421] $/../=35$	$[3^21]$ $/../=21$	$[32^2]$ $/../=21$	$n^M_{\Sigma[\lambda]}$
7	1								1
6	1	1							7
5	2	2	1						28
4	2	3	2	1	1				77
3	3	4	4	1	2	1			161
2	3	5	5	2	3	2	1		266
1	4	6	6	2	4	3	1	1	357
0	4	6	6	3	4	3	2	1	393
Σ	36	47	43	15	24	15	6	3	2197

processes; the Liouvillians $[H,]_-$ involving dominant dipolar, double resonance, zero magnetic field terms, or field cycling techniques, generally do not meet the requisite criteria to be stationary constants of motion.*

4. Concluding remarks

To summarize, it has been shown by analyzing the combinatorial properties of $p \leq 3$ generalized lexical wordlengths and invoking mapping from the GWLs onto the $\mathcal{S}_n$ irrep set that there are direct methods to establish the dual irreps of identical spin-one clusters over M subspaces. For lower $\mathcal{S}_n$ groups of $n \ll 12$, it is not necessary to invoke Racah methods, provided the group algebra or the inner tensor products are known; such ITPs adequately determine the duality of the non-simple reducible space for $[A]_n(\mathcal{S}_n)^{(I_i)}$ clusters.

The present work on higher spin clusters, essentially $I_i = 1$ clusters, exhibits a marked contrast to the nature of spin-1/2 clusters, whose simple reducibility (SR) over operator bases of Liouville space and mapping under $\mathcal{S}_n \times \mathrm{SU2}$ arise from all the distinct υ's within the $\{D^k(\tilde{U}) \times \tilde{\Gamma}^{[\tilde{\lambda}]}(\upsilon)\}$ dual irreps [22], for which υ takes forms involving (111..11), ({111.011}),..,.; the analogous $k_i \leq 2$ recoupling υ span (222..22), ({222.122}), ({222.022}),., ({222.011}),..,.. for instance, before considering the NSR aspect of such bases.

*For a discussion of criteria under which the Hamiltonian belongs to the $[n] \to \mathcal{A}_1$ representations and constitutes a constant of motion, the reader is referred to Corio [30]. However, the use of coherent superpositional opertaor bases, derived analogously to symmetrized tensor bases, may be mathematically convenient, even where the stationary H is not a constant of motion [31,32].

Knowledge of the (scalar) invariants (or constants of motion) under a generalized group, such as SU(n) for the single-spin case [23] and under $\mathcal{S}_n$ for clusters of such SU(n) spins, provides the more fundamental insight into the nature of spin systems. Explicit commutator tables for single-spin problems over Liouville space, i.e. of the form given in ref. [24] and utilized by Reddy and Narasimhan [25], provide little additional insight since their properties are inherent in the invariant algebra under SU(n) generators [23]; the spin dynamics in such Cartesian tensor basis formulations [24,25] are derivable by inspection from suitable expectation values of the more general SO(3) density matrix, as discussed by Santuary and Halstead [26].

Further physical science applications of -tuple number partitions may be found in the work of Mekjian and Lee [27], which appeared whilst the present paper was being reviewed, or in the text by Abhyanker [28]. For our final comments, we return to the masterful mathematical writings on combinatorics of Rota et al. [29] and of Berge [2]. The former point out the existence of an interesting relationship between combinatorics in the form of monomials – maximal product binomial functions – and the umbrial calculus of pattern algebra. Berge, in an illuminating and highly readable classic, recalls various interesting historical aspects to the origins of combinatorics.

Appendix

The $p \leq 3$-tuple inventory for the $[\mathrm{A}]_5(I_i = 1)(\mathcal{S}_5)$ spin cluster takes the form

M	{: :}	{: :} / reordered	/ : . . : /	
5	:5:		1	
4	:41:		5	
3	:32:	:41:	15	(A.1)
2	$:31^2:$	:32:	30	
1	$:2^21:$	:32: , :41:	45	
0	$:2^21:$, $:31^2:$	:5:	51	

For subduction from $\mathcal{S}_5$ to $\mathcal{S}_5 \downarrow C_{4v}$ the $[\lambda]$'s are associated with the mappings

$$\begin{aligned} [41] &\to \mathcal{A}_1 + \mathcal{B}_2 + \mathcal{E}, \\ [32] &\to \mathcal{A}_1 + \mathcal{B}_1 + \mathcal{B}_2 + \mathcal{E}, \\ [31^2] &\to \mathcal{A}_2 + \mathcal{B}_1 + 2\mathcal{E}. \end{aligned} \tag{A.2}$$

The corresponding inventory for the analogous $[\mathrm{A}]_6$ spin-one cluster is given by the expression

$$\{.\}^M = \begin{pmatrix} 1 & 0 & & & & & \\ 0 & 1 & 0 & & \bigcirc & & \\ 0 & 1 & 1 & 0 & & & \\ 0 & 0 & 0 & 1 & 1 & 0 & \\ 0 & 0 & 2 & 0 & 0 & 1 & \\ 0 & 1 & 0 & 0 & 0 & 2 & \\ 1 & 0 & 0 & 1 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} :6: \\ :51: \\ :42: \\ :41^2: \\ :3^2: \\ :321: \\ :2^3: \end{pmatrix}. \tag{A.3}$$

Subduction from S_6 to $S_6 \downarrow O$ symmetry proceeds via the mappings

$$\begin{aligned} [51] &\to \mathrm{E} + \mathrm{T}_1, \\ [42] &\to \mathrm{A}_1 + \mathrm{E} + 2\mathrm{T}_2, \\ [3^2] &\to 2\mathrm{A}_2 + \mathrm{T}_1, \end{aligned} \tag{A.4}$$

with the $p = 3$ partitions yielding the mappings

$$\begin{aligned} [41^2] &\to \mathrm{A}_2 + 2\mathrm{T}_1 + \mathrm{T}_2, \\ [321] &\to 2\mathrm{E} + 2\mathrm{T}_1 + 2\mathrm{T}_2, \\ [2^3] &\to 2\mathrm{A}_1 + \mathrm{T}_2. \end{aligned} \tag{A.5}$$

Under S_7, $S_7 \downarrow \mathrm{D}_5$, subductions over F', spanning unit set $\{\mathrm{A}_1, \mathrm{A}_2, \mathrm{E}_1, \mathrm{E}_2\}$ map onto

$$\begin{aligned} [61] &\to (1, 1, 1, 1)\mathrm{F}', \\ [52] &\to (2, 0, 3, 3)\mathrm{F}', \\ [43] &\to (1, 1, 3, 3)\mathrm{F}', \end{aligned} \tag{A.6}$$

whereas the $p = 3$ partitions map onto

$$[51^2] \to (0, 3, 3, 3)\mathrm{F}', \tag{A.7}$$

$$[421] \to (4, 3, 7, 7)\mathrm{F}', \tag{A.8}$$

$$[3^21] \to (1, 4, 4, 4)\mathrm{F}', \tag{A.9}$$

$$[32^2] \to (4, 1, 4, 4)\mathrm{F}'. \tag{A.10}$$

For sevenfold spin-one cluster, the inventory over $\{|IM.\rangle\}^M$ follows the form of table 1 of the second paper of ref. [4].

Note added in proof

A recent study [33] of Casimir invariants provides a rather concise statement of the importance of the Racah chain for NMR problems which stresses the nature of seniority for dual unitary algebras. Certain fundamental distinctions in the nature of reduced matrix elements associated with NMR spin dualities, i.e. from the accepted forms of Racah algebra for shell models in other areas of physics, are stressed in this work. Such extensions to the application of group theory in NMR stem from the realisation of the underlying role of certain wreath-product aspects of finite symmetries applied to NMR. In addition, the higher unitary algebras, $SU(6) \times \mathcal{S}_n$, (and above) are discussed.

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